

Argonne National Laboratory

**SURFACE AND VOLUME PROPERTIES
OF GROUND STATE NUCLEAR MATTER
IN THE HARTREE-FOCK AND
PUFF-MARTIN APPROXIMATIONS**

by

John C. Reynolds

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Applied Mathematics Division

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ABSTRACT

A method is derived for computing the ground state properties of a spatially inhomogeneous self-bound system of many particles. This method is used to compute the density and effective potential across a plane surface of nuclear matter in the Hartree-Fock approximation and in an approximation developed by R. D. Puff and P. C. Martin which takes into account certain two-body correlation effects.

A general theory of many-particle systems is developed in terms of the n -particle field correlation or Green's functions. It is shown that, for zero temperature and pressure, this treatment may be extended to inhomogeneous systems by replacing the condition of spatial homogeneity on the Green's functions by appropriate asymptotic boundary conditions. Such conditions are derived for a semi-infinite volume of material with a single plane surface.

This development is then applied to nuclear matter in the Hartree-Fock approximation. A solution for homogeneous matter is first obtained. A Gaussian interparticle potential is used, with depth and range fitted to low-energy scattering data. Nuclear saturation is produced by using an admixture of exchange forces. The resulting binding energy per particle is -3.63 Mev, and the interparticle spacing is 1.25 fermi. These may be compared with experimental values of -15.75 Mev and 1.1 to 1.2 fermi.

The inhomogeneous geometry described above is then considered. A short development is made of an approximation analogous to the Thomas-Fermi approximation in atomic physics, but it is shown that this approach breaks down for nuclear matter and leads to inconsistencies because of the exchange nature of the forces. A numerical solution for the inhomogeneous geometry is then obtained by an iterative self-consistent procedure, using an effective mass approximation. The thickness of the resulting surface (the distance over which the density drops from 90 per cent to 10 per cent of its asymptotic value in the interior) is 2.01 compared with an experimental value of 2.5 ± 0.2 fermi, and the density function exhibits oscillations near the surface due to the sharpness of the edge. The effective potential is strongly momentum-dependent but is nearly isotropic.

A similar treatment is carried out for the Puff-Martin approximation. In this approximation the effective potential becomes an energy-dependent function which is expressed as a folding integral of the spectral function of the system and a two-body scattering matrix. An ambiguity in the definition of the pressure appears in the approximation; it is resolved by showing that a pressure expression derived from local-transport considerations must be used to insure the existence of time-independent solutions for the inhomogeneous case.

We follow Puff in using an interparticle potential consisting of a separable Yamaguchi potential plus an S-state repulsive hard shell. In the homogeneous case the approximation leads to a binding energy per particle of -14.4 to -17.5 Mev and an interparticle spacing of 0.871 to 1.01 fermi (depending on which expression for the pressure is set equal to zero to obtain an uncompressed system). A computation of the density correlation function is given.

The inhomogeneous case is again treated by an iterative self-consistent procedure with an effective-mass approximation. The results give a surface thickness of 2.33 fermi and a surface energy of 18.79 Mev, which may be compared with experimental values of 2.5 ± 0.2 fermi and 17.804 Mev. As in the Hartree case, the effective potential is nearly isotropic, but now there are no significant oscillations inside the surface.

CHAPTER I

INTRODUCTION AND GENERAL FORMALISM

I.1. Introduction

One of the central purposes of nuclear physics is the investigation of the many-nucleon problem; ideally, the properties of nuclear systems (beyond the trivial two-particle system) should be derivable from a knowledge of the interparticle potential. At least for the heavier nuclei, one would expect the number of particles in the system to be sufficiently great to allow the use of statistical methods. Unfortunately, this approach is hindered by the existence of the Coulomb repulsion between protons, which dominates the attractive nuclear forces for sufficiently large nuclei and prevents the existence of bound systems of more than a few hundred particles.

To circumvent this difficulty many authors have examined an idealized system, usually called nuclear matter, in which the Coulomb repulsion is removed from the interparticle potential. Under these circumstances macroscopically large bound systems will occur which are easily amenable to statistical methods. Certain properties of actual nuclei, particularly

those which depend smoothly on the number of particles and for which Coulomb effects are either small or analytically removable, should bear a close resemblance to the analogous properties of the idealized nuclear matter.

At present, however, most investigations of nuclear matter have been limited to homogeneous matter, i.e., to the volume properties of macroscopically large systems. In this report we will develop an extension of these investigations to inhomogeneous systems, and in particular to surface properties. This extension greatly increases the scope of the nuclear properties which may be obtained from an examination of nuclear matter.

Our general approach relies upon the description of many-body systems by a set of n -particle field-correlation or Green's functions similar to those introduced by Martin and Schwinger.⁽¹⁾ We shall show that the Green's functions for an inhomogeneous system satisfy the same differential equations as those for a homogeneous system, and that the spatial inhomogeneity is generated by appropriate spatial boundary conditions. In particular, we will obtain the boundary conditions for a semi-infinite volume of material with a single plane surface and present numerical solutions for this geometry using two methods, the Hartree-Fock and the Puff-Martin⁽²⁾ approximations.

The most important property of nuclei which must be reflected by nuclear matter is saturation. Although the nucleus is a system of particles bound by interparticle attraction, the system does not collapse as the number of particles increases. Specifically, the energy per particle and the density of the nucleus (when the effects of Coulomb repulsion are discounted) tend to constant limits for large numbers of particles. This implies that an individual nucleon feels only the potential produced by its close neighbors, i.e., that the interparticle potential is short-ranged, and that some mechanism, such as arising from a repulsive core or exchange effects, prevents the nucleons from packing too closely as the number of particles increases.

This situation is illustrated quantitatively by the Weizsäcker semi-empirical mass formula, which expresses the binding energy of nuclei by a constant binding energy per particle of -15.75 Mev,⁽⁸⁾ modified by terms describing Coulomb repulsion, surface effects, and symmetry energy. One would expect this formula, with the Coulomb term dropped, to describe nuclear matter as well. Similarly, the density of nuclear matter should be qualitatively equal (but somewhat larger since there is no Coulomb repulsion) to the density of large nuclei. Such a situation should also hold for such parameters as the optical potential.

In actually solving the equations which describe nuclear matter, the simplest approximation, which neglects all correlation effects, is the Hartree-Fock approximation. In Chapter II we give a general derivation of this approximation in terms of the Green's-function formalism and describe its solution for homogeneous matter. Chapter III gives the corresponding solution for inhomogeneous matter with a plane surface.

In the Hartree approximation each nucleon moves in an effective potential due to the remaining particles, which is expressed as a folding integral of the interparticle potential and the spectral function of the system (which is, in turn, the product of one-particle wave functions integrated over the degeneracy variable). In the homogeneous case the particles fill a spherical region in momentum space bounded by the Fermi momentum. The principal shortcoming of the approximation is its inability to deal with a repulsive core in the interparticle potential. As a result, saturation must be induced purely by exchange effects, and the resulting system has a binding energy per particle which is only about one-fourth of the Weizsäcker value. For the inhomogeneous case the surface (i.e., the density across the surface) is illustrated in Figure 3.

To overcome the shortcomings of the Hartree method, an approximation must be used which takes into account sufficient correlation effects to allow the use of repulsive cores. In Chapters IV and V we describe the homogeneous and inhomogeneous solutions for an approximation of this type, which was developed by P. C. Martin and originally applied to the homogeneous case by R. D. Puff,⁽²⁾ and which gives excellent agreement with the Weizsäcker binding energy.

This approximation, which we call the Puff-Martin approximation, leads to an energy-dependent effective potential which is a folding integral of the two-particle scattering matrix and the spectral function. In the homogeneous case the particles still occupy a region of momentum space with a sharp cut-off at the Fermi momentum, but the energy dependence of the effective potential leads to a reduction of the density within this region, so that the Fermi momentum for a given total density is greater in this approximation than in the Hartree case. The resulting density across the surface in the inhomogeneous case is given in Figure 16.

It should be noted that the calculations for the Puff-Martin approximation, which are discussed in Chapters IV and V, have been reported elsewhere by R. D. Puff and the present author.^(3,4) Our present purpose is to give a more detailed account of the derivations and numerical techniques involved in these calculations.

1.2. The Many-particle Green's Functions

The properties of a many-particle system such as nuclear matter are conveniently expressed by a set of field correlation functions or Green's

functions, which are the expectation values of time-ordered products of the field operators of the system. In this section we define these Green's functions, obtain the differential equations and boundary conditions which they must satisfy, and show how the ground state properties of a system may be extracted from the Green's functions. A more extensive discussion of these derivations is given in Reference 1.

The nuclear particles are described by field operators $\psi(\xi \mathbf{r} t)$, where the discrete variable ξ describes spin and isotopic spin. In most of our derivations we will omit any explicit mention of the ξ -variable by using the convention that the variable \mathbf{r} actually represents both ξ and \mathbf{r} . To further simplify our equations we assume a system of units in which $\hbar = 1$.

Since the nucleons are Fermi-Dirac particles, the field operators for equal times obey the anticommutation relations

$$\begin{aligned}\psi(\mathbf{r}_1 t) \psi(\mathbf{r}_2 t) + \psi(\mathbf{r}_2 t) \psi(\mathbf{r}_1 t) &= 0 \\ \psi^+(\mathbf{r}_1 t) \psi^+(\mathbf{r}_2 t) + \psi^+(\mathbf{r}_2 t) \psi^+(\mathbf{r}_1 t) &= 0 \\ \psi(\mathbf{r}_1 t) \psi^+(\mathbf{r}_2 t) + \psi^+(\mathbf{r}_2 t) \psi(\mathbf{r}_1 t) &= \delta(\mathbf{r}_1 - \mathbf{r}_2)\end{aligned}\quad (1.1)$$

The time development of the ψ 's is determined by a generalized Hamiltonian

$$H = H - \mu N \quad , \quad (1.2)$$

where H is the usual Hamiltonian

$$\begin{aligned}H = & - \int (d\mathbf{r}) \psi^+(\mathbf{r} t) \frac{\nabla^2}{2m} \psi(\mathbf{r} t) + \frac{1}{2} \int (d\mathbf{r}_1)(d\mathbf{r}_2)(d\mathbf{r}'_1)(d\mathbf{r}'_2) \psi^+(\mathbf{r}_1 t) \psi^+(\mathbf{r}_2 t) \quad ; \\ & \times \langle \mathbf{r}_1 \mathbf{r}_2 | v | \mathbf{r}'_1 \mathbf{r}'_2 \rangle \psi(\mathbf{r}'_2 t) \psi(\mathbf{r}'_1 t) \quad ,\end{aligned}\quad (1.3)$$

N is the number operator

$$N = \int (d\mathbf{r}) \psi^+(\mathbf{r} t) \psi(\mathbf{r} t) \quad , \quad (1.4)$$

and μ is a numerical parameter which may be identified with the thermodynamic chemical potential. The additional term $-\mu N$ in the generalized Hamiltonian is equivalent to the presence of a constant external potential and merely introduces a constant phase factor in the field operators. We have introduced this term in order to produce an eventual simplification of the boundary conditions on the Green's functions.

The equation of motion for the field operators is $i \frac{\partial}{\partial t} \psi = \psi H - H \psi$, which has the explicit form

$$\left[i \frac{\partial}{\partial t} + \mu + \frac{\nabla_1^2}{2m} \right] \psi(r_1 t) - \int (dr_2)(dr'_1)(dr'_2) \psi^\dagger(r_2 t) \langle r_1 r_2 | v | r'_1 r'_2 \rangle \psi(r'_2 t) \psi(r'_1 t) = 0 \quad (1.5)$$

We now define a set of n-particle Green's operators G_n by

$$G_n(r_1 t_1 \dots r_n t_n; r'_1 t'_1 \dots r'_n t'_n) = (-i)^n \epsilon(t_1 \dots t_n; t'_1 \dots t'_n) (\psi(r_1 t_1) \dots \psi(r_n t_n) \psi^\dagger(r'_n t'_n) \dots \psi^\dagger(r'_1 t'_1))_+ \quad (1.6)$$

The symbol $()_+$ indicates a time-ordering of the field operators with the earliest time to the right. The quantity ϵ is the antisymmetric function $(-1)^p$, where p is the number of permutations necessary to convert the time-ordered sequence of t 's into the standard sequence $t_1 \dots t_n; t'_1 \dots t'_n$. The presence of ϵ , along with the anticommutation relations (1.1), removes the time-ordering discontinuities at the points $t_i = t_j$ and $t'_i = t'_j$, but not at the points $t_i = t'_j$.

A set of coupled differential equations for the Green's operators may be obtained by differentiating (1.6) with respect to t_1 and applying (1.5). A set of delta-function terms arises from the discontinuities as t_1 crosses each of the t'_j . The resulting equations are

$$\begin{aligned} & \left[i \frac{\partial}{\partial t_1} + \mu + \frac{\nabla_1^2}{2m} \right] G_n(r_1 t_1 \dots r_n t_n; r'_1 t'_1 \dots r'_n t'_n) + i \int (dr_{n+1})(d\bar{r}_1)(d\bar{r}_{n+1}) \langle r_1 r_{n+1} | v | \bar{r}_1 \bar{r}_{n+1} \rangle \\ & G_{n+1}(\bar{r}_1 t_1 r_2 t_2 \dots r_n t_n \bar{r}_{n+1} t_1; r'_1 t'_1 \dots r'_n t'_n r'_{n+1} t'_1) = \\ & \sum_{j=1}^n (-1)^{j-1} \delta(r_1 - r'_j) \delta(t_1 - t'_j) G_{n-1}(r_2 t_2 \dots r_n t_n; r'_1 t'_1 \dots r'_{j-1} t'_{j-1} r'_{j+1} t'_{j+1} \dots r'_n t'_n) \end{aligned} \quad (1.7)$$

where $G_0 = 1$.

The Green's functions are simply expectation values of the Green's operators:

$$G_n \text{ function} = \langle G_n \text{ operator} \rangle \quad (1.8)$$

The differential equations (1.7) will hold as written for the Green's functions providing that the expectation value is normalized so that $G_0 = \langle 1 \rangle = 1$. To complete the specification of the Green's functions we make the particular choice of the expectation value

$$\langle X \rangle = \frac{\text{Tr} X e^{-i(H-\mu N)\tau}}{\text{Tr} e^{-i(H-\mu N)\tau}} = \frac{\sum_{N,E} e^{-i(E-\mu N)\tau} \sum_{\gamma} \langle N E \gamma | X | N E \gamma \rangle}{\sum_{N,E} e^{-i(E-\mu N)\tau} \sum_{\gamma} 1} \quad (1.9)$$

where N , E , and γ are the eigenvalues of the number operator, energy, and degeneracy variables, respectively, and where the number τ has a negative imaginary part to produce convergence.

The advantage of this particular choice of the expectation value lies in the simple boundary conditions which result from the cyclical properties of the trace. For example, suppose τ is real (with an infinitesimal negative imaginary part), and all the variables t_i and t'_i are within the range 0 to τ . Then consider G_n for $t_1 = 0$:

$$G_n(r_1 0 r_2 t_2 \dots r_n t_n; r'_1 t'_1 \dots r'_n t'_n) = (-i)^n \epsilon(0 t_2 \dots t_n; t'_n \dots t'_1) \times \frac{\text{Tr} \left[e^{-iH\tau} (\psi(r_2 t_2) \dots \psi(r_n t_n) \psi^\dagger(r'_n t'_n) \dots \psi^\dagger(r'_1 t'_1))_+ \psi(r_1 0) \right]}{\text{Tr} e^{-iH\tau}} \quad (1.10)$$

and for $t_1 = \tau$,

$$G_n(r_1 \tau r_2 t_2 \dots r_n t_n; r'_1 t'_1 \dots r'_n t'_n) = (-i)^n \epsilon(\tau t_2 \dots t_n; t'_n \dots t'_1) \times \frac{\text{Tr} \left[e^{-iH\tau} \psi(r_1 \tau) (\psi(r_2 t_2) \dots \psi(r_n t_n) \psi^\dagger(r'_n t'_n) \dots \psi^\dagger(r'_1 t'_1))_+ \right]}{\text{Tr} e^{-iH\tau}} \quad (1.11)$$

The cyclical property of the trace allows us to move $\psi(r_1 0)$ in (1.10) to the left end of the expression in square brackets. Then, by using the integral equation of motion:

$$\psi(r_1 \tau) = e^{iH\tau} \psi(r_1 0) e^{-iH\tau}, \quad (1.12)$$

we may show that

$$G_n(r_1 \tau r_2 t_2 \dots r_n t_n; r'_1 t'_1 \dots r'_n t'_n) = \frac{\epsilon(\tau t_2 \dots t_n; t'_n \dots t'_1)}{\epsilon(0 t_2 \dots t_n; t'_n \dots t'_1)} G_n(r_1 0 r_2 t_2 \dots r_n t_n; r'_1 t'_1 \dots r'_n t'_n) = -G_n(r_1 0 r_2 t_2 \dots r_n t_n; r'_1 t'_1 \dots r'_n t'_n), \quad (1.13)$$

since $2n-1$ permutations are required to carry the numerator of ϵ/ϵ into the denominator. A similar boundary condition holds for each of the time variables t_i and t'_i .

To make use of these Green's functions, we must be able to extract the expectation values for a given energy and number of particles (averaged over the degeneracy variable) from the weighted sum in (1.9). A detailed discussion of this procedure for arbitrary values of E is given by Martin and Schwinger.⁽¹⁾ In dealing with nuclear matter, however, we are only

interested in the ground states $E = E_0(N)$ (where E_0 is the lowest energy level of a system of N particles), and for these states the extraction is straightforward.

We need only take the limit of (1.9) as $i\tau \rightarrow \infty$ (thermodynamically, this corresponds to zero temperature). The sum in (1.9) then reduces to the desired expectation value

$$\langle X \rangle \xrightarrow[i\tau \rightarrow \infty]{\text{Average over } \gamma} \langle N_0 E_0(N_0) \gamma | X | N_0 E_0(N_0) \gamma \rangle, \quad (1.14)$$

where N_0 is the value of N for which the function $E_0(N) - \mu N$ is a minimum. Thus, to obtain ground-state expectation values we must first obtain formal expressions for the Green's functions which incorporate the boundary conditions and then take the limit as $i\tau \rightarrow \infty$, adjusting μ to give the desired value of N_0 .

The number of particles, N_0 , is a function of μ which is determined by minimizing the function $E_0(N) - \mu N$. For a system of macroscopic size we may treat N as a continuous variable and minimize this function by setting its derivative at $N = N_0$ equal to zero, obtaining

$$\mu = \left. \frac{dE_0}{dN} \right|_{N=N_0}. \quad (1.15)$$

For this point to be a minimum we must also have

$$\left. \frac{d^2}{dN^2} [E_0(N) - \mu N] \right|_{N=N_0} = \left. \frac{d^2 E_0}{dN^2} \right|_{N=N_0} > 0. \quad (1.16)$$

Actually, this is an oversimplification. The function $E_0(N) - \mu N$ may have one or more local minima which satisfy (1.15) and (1.16), and the values of the function at these points may or may not be less than the value $E_0(N) - \mu N = 0$ at the end point $N = 0$. Furthermore, the true minimum N_0 may jump discontinuously from one local minimum to another or to the end point as μ is varied.

We limit ourselves to the case of a single local minimum. For large μ , the true minimum $N_0(\mu)$ will be the local minimum and will satisfy (1.15) and (1.16), but for sufficiently negative μ the true minimum will be the end point $N_0(\mu) = 0$. Let $N_{\text{crit}}, \mu_{\text{crit}}$ be the point at which the local minimum ceases to be the true minimum. This point satisfies (1.15). In addition,

$$\left. E_0(N) - \mu N \right|_{\substack{\mu = \mu_{\text{crit}} \\ N = N_{\text{crit}}}}$$

must have the same value as it has for $N = 0$:

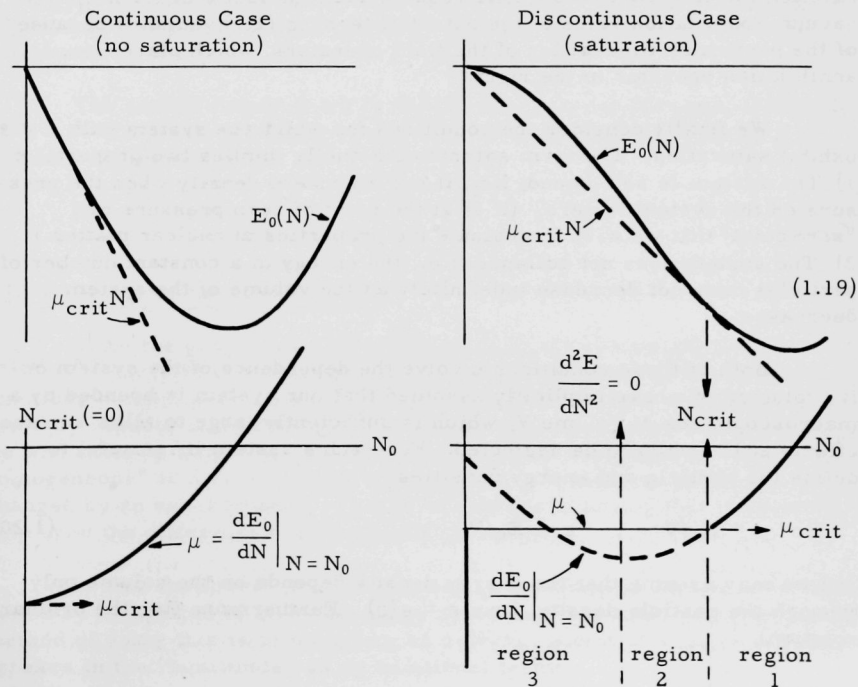
$$E_0(N_{\text{crit}}) - \mu_{\text{crit}} N_{\text{crit}} = E_0(N) - \mu N \Big|_{N=0} = 0 \quad (1.17)$$

Thus, this point is determined by

$$\mu_{\text{crit}} = \frac{dE_0}{dN} \Big|_{N=N_{\text{crit}}} = \frac{E_0(N_{\text{crit}})}{N_{\text{crit}}} \quad (1.18)$$

and $N_0(\mu)$ will be discontinuous at this point if $N_{\text{crit}} > 0$. It will turn out that the existence of this discontinuity is a necessary condition for saturation.

The following diagram illustrates the two cases of continuous and discontinuous $N_0(\mu)$:



In region 1 of the figure for the discontinuous case the local extremum is the true minimum, in region 2 it is a local minimum but not the true minimum, and in region 3 it is a local maximum.

The actual solution of the Green's-function equations will not explicitly exhibit a discontinuity of this sort. Instead, the equations will possess two distinct solutions (within a region of μ containing the point of discontinuity): an ordinary finite-density solution for which $\mu = dE_0/dN$, and an extraordinary vacuum solution for $N = 0$. The discontinuity must be imposed by switching from the ordinary to the extraordinary solution at $\mu = \mu_{\text{crit}}$. In practice, one normally considers only values of μ which are larger or equal to μ_{crit} , and the extraordinary solution is ignored. However, an explicit consideration of this discontinuity will be necessary to justify our derivation of the equations for inhomogeneous matter.

The extraordinary vacuum solution is simply $\langle N = 0 \mid G_n \mid N = 0 \rangle$. It is useful to note that the one-particle vacuum Green's function G_1 is independent of the interparticle potential and is equal to the analogous function for free particles. This results from the fact that for $n = 1$ the vacuum expectation value of the potential term in (1.7) vanishes because of the particular time-order of the field operators, which places an annihilation operator to the right.

We finally consider the conditions for which the system will exhibit saturation. The term saturation actually implies two properties:

- 1) The system is self-bound, i.e., it has a nonzero density when the pressure on the system is zero. (It is at the point of zero pressure or "zero point" that we wish to evaluate the properties of nuclear matter.)
- 2) The system does not collapse, i.e., the energy of a constant number of particles does not decrease indefinitely as the volume of the system decreases.

Both of these conditions involve the dependence of the system on its volume. We have implicitly assumed that our system is bounded by a macroscopic box of volume V , which is sufficiently large to allow surface effects at the walls to be neglected. For such a system it is useful to define the particle and energy densities

$$\rho = N_0/V \quad ; \quad \epsilon = E_0/V \quad , \quad (1.20)$$

and we may assume that the energy density depends on the volume only through the particle density, i.e., $\epsilon = \epsilon(\rho)$. Furthermore (for the ordinary solution),

$$\mu = \frac{d\epsilon(\rho)}{d\rho} \quad . \quad (1.21)$$

With the use of the function $\epsilon(\rho)$ the energy may be written as an explicit function of the number of particles and the volume:

$$E_0 = V\epsilon(N_0/V) \quad (1.22)$$

From this equation we may obtain an expression for the pressure by using the thermodynamic definition of pressure as the negative rate of change of the energy of the system with respect to its volume, with the number of particles held constant. This gives

$$P = - \left(\frac{\partial E_0}{\partial V} \right)_N = \rho \frac{d\epsilon}{d\rho} - \epsilon(\rho) \quad (1.23)$$

or, by means of (1.21),

$$P = \rho\mu - \epsilon \quad (1.24)$$

From this we see that the zero-pressure point is just the point $N_0 = N_{\text{crit}}$, $\mu = \mu_{\text{crit}}$, and the first requirement for saturation, that the density be nonzero at this point, is equivalent to requiring that $N_0(\mu)$ or $\rho(\mu)$ be discontinuous at this point.

The second requirement is that (1.22) must not decrease indefinitely as $V \rightarrow 0$. This will not occur if $\epsilon(\rho)$ increases at least linearly as $\rho \rightarrow \infty$, which is equivalent to

$$\lim_{\rho \rightarrow \infty} \frac{d\epsilon}{d\rho} = \lim_{\rho \rightarrow \infty} \mu(\rho) \geq 0 \quad (1.25)$$

I.3. Inhomogeneous-case Methods

Since the generalized Hamiltonian (1.2) and the weight factor $e^{-i(H-\mu N)\tau}$ in (1.9) are translationally invariant operators, the Green's functions defined in Section I.2 are spatially homogeneous functions and are only capable of describing infinite homogeneous matter. In general, we will refer to a function of one or more spatial variables as "spatially homogeneous" if it is unchanged when all of its spatial variables are changed by an equal amount. This is equivalent to saying that it depends only upon the differences of its spatial variables.

In this section we wish to generalize the Green's functions so that they may be applied to inhomogeneous systems. The most straightforward method of doing this is to introduce an external potential $V_{\text{ext}}(\mathbf{r})$, which appears in the Hamiltonian as an additional term:

$$H_{\text{ext}} = \int (d\mathbf{r}) V_{\text{ext}}(\mathbf{r}) \psi^\dagger(\mathbf{r}t) \psi(\mathbf{r}t) \quad (1.26)$$

The introduction of this potential modifies the differential equations for the Green's functions by changing the differential operator in the first line of (1.7) to

$$\left[i \frac{\partial}{\partial t_1} + \mu - V_{\text{ext}}(r_1) + \frac{\nabla_1^2}{2m} \right] . \quad (1.27)$$

In order to examine the surface of nuclear matter, we may localize the matter by introducing a potential well, or, equivalently, a potential barrier. Furthermore, if we choose $\mu = \mu_{\text{crit}}$ to give zero pressure and the well has macroscopic dimensions, we would expect an infinitesimal potential to be sufficient to produce the localization, since there will be no back pressure against the well and since a macroscopic well will have an infinitesimal zero-point energy. On the other hand, such an infinitesimal well would not have any distorting effect on the structure of the nuclear surface.

To realize this situation mathematically we introduce a sharp-edged, infinitesimal well in the macroscopic region R_0 , by using the external potential

$$V_{\text{ext}}(r) = \begin{cases} -\epsilon, & \text{if } r \text{ in } R_0 \\ \epsilon, & \text{if } r \text{ not in } R_0 \end{cases} , \quad (1.28)$$

where ϵ is positive. The effects of such a potential may be inferred directly from (1.27). Since $V_{\text{ext}}(r)$ is additive to $\mu = \mu_{\text{crit}}$, the local properties of the system, at macroscopic distances from the surface of R_0 , will be the same as the properties of a homogeneous system for $\mu = \mu_{\text{crit}} + \epsilon$ inside the well, and $\mu = \mu_{\text{crit}} - \epsilon$ outside the well.

The ability of this infinitesimal well to localize the system stems mathematically from the discontinuity of $\rho(\mu)$ at $\mu = \mu_{\text{crit}}$, which occurs for a saturated system. Inside the well, for $\mu = \mu_{\text{crit}} + \epsilon$ we have matter at the zero-pressure density $\rho = N_{\text{crit}}/V$, whereas outside the well, for $\mu = \mu_{\text{crit}} - \epsilon$, we have a vacuum: $\rho = 0$.

The essence of this procedure is that the external potential, being infinitesimal, is a purely formal entity which need not be inserted explicitly into the Green's-function equations. The inhomogeneous-case Green's functions satisfy the same equations as the homogeneous functions. The only change is that the condition of spatial homogeneity must be replaced by spatial boundary conditions which specify that the local properties of the system approach the properties of saturated homogeneous matter inside the region R_0 and approach the properties of the vacuum outside R_0 . These local properties include the Green's functions G_n themselves, which are local properties of their average spatial coordinate $R = (1/2n)(r_1 + \dots + r_n + r'_1 + \dots + r'_n)$.

The simplest possible inhomogeneous geometry is that of a single plane surface of matter localized by choosing R_0 to be the half-space $Z > 0$. In this case, the local properties of the system are spatially inhomogeneous only along the Z -axis, approaching the properties of homogeneous matter as $z \rightarrow +\infty$ and of the vacuum as $z \rightarrow -\infty$. In the following chapters we will obtain solutions for inhomogeneous nuclear matter (in the Hartree-Fock and Puff-Martin approximations) in this semi-infinite geometry.

CHAPTER II

THE HARTREE-FOCK APPROXIMATION IN THE HOMOGENEOUS CASE

II.1. General Derivation

In Chapters II and III we derive the uncorrelated or Hartree-Fock approximation and obtain solutions for both the homogeneous and inhomogeneous cases. We refer to this as the Hartree-Fock approximation by analogy with the case of atomic systems, in which it leads to the conventional Hartree-Fock equations for the one-particle wave functions. Although this approximation is known to be severely inadequate for dealing with nuclear matter, it will be useful to develop its consequences, particularly in the inhomogeneous case, as a preliminary to investigating correlation effects.

The Green's function G_1 satisfies the differential equation

$$\left[i \frac{\partial}{\partial t_1} + \mu + \frac{\nabla_1^2}{2m} \right] G_1(r_1 t_1; r_1' t_1') + i \int (dr_2)(dr_1'') (dr_2') \langle r_1 r_2 | v | r_1'' r_2' \rangle G_2(r_1'' t_1 r_2 t_1; r_1' t_1' r_2' t_1') = \delta(r_1 - r_1') \delta(t_1 - t_1') \quad (2.1)$$

along with the appropriate periodic boundary conditions in time. In the Hartree-Fock approximation we neglect all correlation effects and replace G_2 by a product of G_1 's, arranged to give the appropriate antisymmetry:

$$G_2(r_1 t_1 r_2 t_2; r_1' t_1' r_2' t_2') \cong G_1(r_1 t_1; r_1' t_1') G_1(r_2 t_2; r_2' t_2') - G_1(r_1 t_1; r_2' t_2') G_1(r_2 t_2; r_1' t_1') \quad (2.2)$$

The substitution of (2.2) into (2.1) then yields

$$\left[i \frac{\partial}{\partial t_1} + \mu + \frac{\nabla_1^2}{2m} \right] G_1(r_1 t_1; r_1' t_1') - \int (dr_1'') V(r_1 r_1'') G_1(r_1'' t_1; r_1' t_1') = \delta(r_1 - r_1') \delta(t_1 - t_1') \quad (2.3)$$

where

$$V(r_1 r_1') = -i \int (dr_2)(dr_2') \left[\langle r_1 r_2 | v | r_1' r_2' \rangle - \langle r_1 r_2 | v | r_2' r_1' \rangle \right] G_1(r_2 t_1; r_2' t_1') \quad (2.4)$$

At this point it is necessary to examine the explicit consequences of the spin and isotopic spin variables which have been compressed into the space coordinates. We assume that the Hamiltonian of the system conserves the total spin and isotopic spin and is symmetric in these variables, i.e., that there is no spin-orbit coupling or electromagnetic effects. Now G_1 is a sum of diagonal elements of the form $\langle | \psi(\xi_1 r_1 t_1) \psi^\dagger(\xi_1' r_1' t_1') | \rangle$. The conservation of the ξ -variables implies that $G_1 = 0$ when $\xi_1 \neq \xi_1'$. In addition, from the definition of G , in terms of

$\text{Tr}(\psi(\zeta_1 r_1 t_1) \psi^\dagger(\zeta_1' r_1' t_1'))_+$, we can see that the symmetry of the Hamiltonian implies that G_1 is independent of ζ_1 when $\zeta_1 = \zeta_1'$. These results allow us to factor out the ζ -dependence:

$$G_1(\zeta_1 r_1 t_1; \zeta_1' r_1' t_1') = \delta_{\zeta_1 \zeta_1'} G_1(r_1 t_1; r_1' t_1') \quad (2.5)$$

By substituting this into (2.3) and (2.4) we find that (2.3) holds as written for the new G_1 , whereas (2.4) becomes

$$\begin{aligned} V(r_1 r_1') &= V(\zeta_1 r_1 \zeta_1' r_1') \\ &= -i \int (dr_2) (dr_2') \left[\sum_{\zeta_2} \left(\langle \zeta_1 r_1 \zeta_2 r_2 | v | \zeta_1 r_1' \zeta_2 r_2' \rangle - \langle \zeta_1 r_1 \zeta_2 r_2 | v | \zeta_2 r_2' \zeta_1 r_1' \rangle \right) \right] \\ &\quad \times G_1(r_2 t_1; r_2 t_1') \quad (2.6) \end{aligned}$$

We assume that the interparticle potential is a sum of products of spatial functions and the possible combinations of the spin exchange operator P^σ and the isotopic-spin exchange operator P^τ :

$$\begin{aligned} \langle \zeta_1 r_1 \zeta_2 r_2 | v | \zeta_1' r_1' \zeta_2' r_2' \rangle &= \langle r_1 r_2 | v_0 | r_1' r_2' \rangle \langle \zeta_1 \zeta_2 | 1 | \zeta_1' \zeta_2' \rangle \\ &+ \langle r_1 r_2 | v_\sigma | r_1' r_2' \rangle \langle \zeta_1 \zeta_2 | P^\sigma | \zeta_1' \zeta_2' \rangle + \langle r_1 r_2 | v_\tau | r_1' r_2' \rangle \langle \zeta_1 \zeta_2 | P^\tau | \zeta_1' \zeta_2' \rangle \\ &+ \langle r_1 r_2 | v_{\sigma\tau} | r_1' r_2' \rangle \langle \zeta_1 \zeta_2 | P^\sigma P^\tau | \zeta_1' \zeta_2' \rangle \quad (2.7) \end{aligned}$$

Let j be the spin coordinate and k the isotopic spin coordinate. Then

$$\begin{aligned} \langle j_1 k_1 j_2 k_2 | P^\sigma | j_1' k_1' j_2' k_2' \rangle &= \delta_{j_1 j_2'} \delta_{j_2 j_1'} \delta_{k_1 k_1'} \delta_{k_2 k_2'} \quad , \\ \langle j_1 k_1 j_2 k_2 | P^\tau | j_1' k_1' j_2' k_2' \rangle &= \delta_{j_1 j_1'} \delta_{j_2 j_2'} \delta_{k_1 k_2'} \delta_{k_2 k_1'} \quad (2.8) \end{aligned}$$

If we substitute this into (2.7) and the result into (2.6), we obtain

$$V(r_1 r_1') = -i \int (dr_2) (dr_2') [\langle r_1 r_2 | v | r_1' r_2' \rangle - \langle r_1 r_2 | v_{\text{ex}} | r_2' r_1' \rangle] G_1(r_2 t_1; r_2 t_1') \quad (2.9)$$

where

$$\begin{aligned} \langle |v| \rangle &= 4 \langle |v_0| \rangle + 2 \langle |v_\sigma| \rangle + 2 \langle |v_\tau| \rangle + \langle |v_{\sigma\tau}| \rangle \quad , \\ \langle |v_{\text{ex}}| \rangle &= \langle |v_0| \rangle + 2 \langle |v_\sigma| \rangle + 2 \langle |v_\tau| \rangle + 4 \langle |v_{\sigma\tau}| \rangle \quad (2.10) \end{aligned}$$

The Green's function G_1 is now specified by equations (2.3), (2.9), (2.10), and the time boundary conditions. These equations may be re-written in a manner which incorporates the boundary conditions by expressing G_1 in a spectral form. Consider the functions $G_>$ and $G_<$, defined analogously to G_1 but without the time ordering:

$$G_{>}(rt; r't') = \frac{1}{i} \langle \psi(rt) \psi^\dagger(r't') \rangle ;$$

$$G_{<}(rt; r't') = -\frac{1}{i} \langle \psi^\dagger(r't') \psi(rt) \rangle . \quad (2.11)$$

Both $G_{>}$ and $G_{<}$ satisfy an equation similar to (2.3) but without the inhomogeneous delta-function term which arose from the time-ordering discontinuity. The Green's function G_1 may be expressed in terms of these functions as

$$G_1(rt; r't') = \begin{cases} G_{>}(rt; r't') & ; \quad t > t' \\ G_{<}(rt; r't') & ; \quad t < t' \end{cases} . \quad (2.12)$$

Now, the considerations which lead to the boundary conditions on G_1 show that

$$G_{<}(rt; r't') = -G_{>}(rt+\tau; r't') . \quad (2.13)$$

These functions depend only upon the time difference $t - t'$. If we introduce their Fourier transforms in this variable,⁽⁵⁾

$$G_{>,<}(rt; r't') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} e^{-i(\omega-\mu)(t-t')} g_{>,<}(rr'\omega) , \quad (2.14)$$

we find by transforming (2.13) that $g_{>}$ and $g_{<}$ are proportional:

$$g_{<}(rr'\omega) = -e^{-i(\omega-\mu)\tau} g_{>}(rr'\omega) . \quad (2.15)$$

Because of this proportionality relationship, which is equivalent to the original boundary conditions on G_1 , we may introduce a single function $A(rr'\omega)$, called the spectral function, such that

$$g_{>}(rr'\omega) = \frac{A(rr'\omega)}{1 + e^{-i(\omega-\mu)\tau}} ; \quad g_{<}(rr'\omega) = \frac{-A(rr'\omega)}{1 + e^{i(\omega-\mu)\tau}} . \quad (2.16)$$

By substituting this into (2.14) and the result into (2.12), we find⁽⁵⁾

$$G(rt; r't') = \frac{1}{i} \int \frac{d\omega}{2\pi} e^{-i(\omega-\mu)(t-t')} \left\{ \begin{aligned} & \frac{A(rr'\omega)}{1 + e^{-i(\omega-\mu)\tau}} ; \quad t > t' \\ & - \frac{A(rr'\omega)}{1 + e^{i(\omega-\mu)\tau}} ; \quad t < t' \end{aligned} \right. \quad (2.17)$$

The functions $g_{>}$ and $g_{<}$ both must satisfy the Fourier transform of the homogeneous equation corresponding to (2.3). Since A is proportional to $g_{>}$ and $g_{<}$, it also satisfies this equation:

$$\left[\omega + \frac{\nabla_1^2}{2m} \right] A(\mathbf{r}_1 \mathbf{r}_1' \omega) - \int (d\mathbf{r}_1'') V(\mathbf{r}_1 \mathbf{r}_1'') A(\mathbf{r}_1'' \mathbf{r}_1' \omega) = 0 \quad . \quad (2.18)$$

[The purpose of writing the transformed variable in (2.14) as $\omega - \mu$ was to eliminate μ from (2.18).]

The form of the inhomogeneous term in (2.3) places a condition on A. If we integrate (2.3) over time across the delta function and substitute (2.17), we find

$$\int \frac{d\omega}{2\pi} A(\mathbf{r} \mathbf{r}' \omega) = \delta(\mathbf{r} - \mathbf{r}') \quad . \quad (2.19)$$

Equation (2.18) has the form of a nonlocal Schroedinger equation, and it possesses wave-function solutions $\psi(\omega \xi \mathbf{r})$, where ξ are the constants of motion necessary to remove degeneracy. We may interpret V as the effective potential on a single particle due to the remaining particles, and the ψ 's as the single-particle wave functions. In terms of the ψ 's the function A may be expressed as

$$A(\mathbf{r} \mathbf{r}' \omega) = \sum_{\xi} \psi(\mathbf{r} \xi \omega) \psi^*(\mathbf{r}' \xi \omega) \quad (2.20)$$

(where the summation over ξ may actually be an integration). Equation (2.19) becomes the completeness relation

$$\int \frac{d\omega}{2\pi} \sum_{\xi} \psi(\mathbf{r} \xi \omega) \psi^*(\mathbf{r}' \xi \omega) = \delta(\mathbf{r} - \mathbf{r}') \quad , \quad (2.21)$$

which specifies the normalization of the wave functions. Such a decomposition will be necessary in the solution of the inhomogeneous case, but the homogeneous case may be treated more directly by Fourier transformation.

To complete the replacement of G_1 by A, we substitute (2.17) into (2.9), obtaining

$$V(\mathbf{r}_1 \mathbf{r}_1') = \int (d\mathbf{r}_2) (d\mathbf{r}_2') \left[\langle \mathbf{r}_1 \mathbf{r}_2 | V | \mathbf{r}_1' \mathbf{r}_2' \rangle - \langle \mathbf{r}_1 \mathbf{r}_2 | V_{\text{ex}} | \mathbf{r}_2' \mathbf{r}_1' \rangle \right] \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A(\mathbf{r}_2' \mathbf{r}_2 \omega)}{1 + e^{+i(\omega - \mu)\tau}} \quad . \quad (2.22)$$

In the low-temperature limit, $i\tau \rightarrow \infty$ and

$$\frac{1}{1 + e^{i(\omega - \mu)\tau}} \rightarrow \eta_{-}(\omega - \mu) \quad \text{where} \quad \eta_{-}(\omega - \mu) = \begin{cases} 0; \omega > \mu \\ 1; \omega < \mu \end{cases} \quad , \quad (2.23)$$

so that (2.22) reduces to

$$V(r_1 r_1') = \int (dr_2)(dr_2') [\langle r_1 r_2 | v | r_1' r_2' \rangle - \langle r_1 r_2 | v_{\text{ex}} | r_2' r_1' \rangle] \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(r_2' r_2 \omega) \quad (2.24)$$

Now the matrix elements of v and v_{ex} may be written as

$$\langle r_1 r_2 | v | r_1' r_2' \rangle = \delta \left(\frac{r_1 + r_2}{2} - \frac{r_1' + r_2'}{2} \right) v(r_1 - r_2, r_1' - r_2') \quad (2.25)$$

(similarly for v_{ex})

In our further work with the Hartree approximation we will limit ourselves to a local interparticle potential. In this case,

$$\langle r_1 r_2 | v | r_1' r_2' \rangle = \delta(r_1 - r_1') \delta(r_2 - r_2') v(r_1 - r_2) \quad (2.26)$$

(similarly for v_{ex})

and (2.24) reduces to

$$V(r_1 r_1') = \delta(r_1 - r_1') \int (dr_2) v(r_1 - r_2) \left\{ \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(r_2 r_2 \omega) \right\} - v_{\text{ex}}(r_1 - r_1') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(r_1 r_1' \omega) \quad (2.27)$$

The bracketed term may be identified with the density $\rho(r_2)$, since this quantity is

$$\rho(r) = \langle \rho(r) \rangle = \langle \psi^\dagger(r) \psi(r) \rangle = \frac{1}{i} G_1(r; r, t^+) \quad (2.28)$$

Substitution of (2.17) and (2.23) gives

$$\rho(r) = \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(r r \omega) \quad (2.29)$$

More precisely, this function is $\rho(\xi r)$, the density of particles of a given spin and isotopic spin. The total density is $4\rho(r)$. Equation (2.27) now permits a further interpretation of V as the effective potential. The first term is a local potential given by the convolution of the interparticle potential with the density; the second is a nonlocal term arising from exchange effects.

In addition to the particle density, we may obtain the energy density. The total energy is

$$E = \langle H \rangle$$

$$\begin{aligned} &= \langle - \int (dr) \psi^\dagger(r) \frac{\nabla^2}{2m} \psi(r) + \frac{1}{2} \int (dr_1)(dr_2)(dr_1')(dr_2') \psi^\dagger(r_1) \psi^\dagger(r_2) \langle r_1 r_2 | v | r_1' r_2' \rangle \psi(r_2') \psi(r_1') \rangle \\ &= -i \int (dr) \lim_{\substack{t' \rightarrow t \\ r' \rightarrow r}} \left(-\frac{\nabla^2}{2m} \right) G_1(rt; r't') - \frac{1}{2} \int (dr_1)(dr_2)(dr_1')(dr_2') \langle r_1 r_2 | v | r_1' r_2' \rangle G_2(r_1 t r_2' t; r_1 t' r_2 t') \end{aligned} \quad (2.30)$$

The use of (2.1) to remove G_2 gives

$$E = -\frac{i}{2} \int (dr) \lim_{\substack{t' \rightarrow t \\ r' \rightarrow r}} \left[i \frac{\partial}{\partial t} + \mu - \frac{\nabla^2}{2m} \right] G_1(rt; r't') \quad (2.31)$$

Since this is an integral over space, the energy density (E/V in the homogeneous case) is

$$\epsilon(r) = -\frac{i}{2} \lim_{\substack{t' \rightarrow t \\ r' \rightarrow r}} \left[i \frac{\partial}{\partial t} + \mu - \frac{\nabla^2}{2m} \right] G_1(rt; r't') \quad (2.32)$$

The substitution of (2.17) and (2.23) reduces this to

$$\epsilon(r) = \frac{1}{2} \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \lim_{r' \rightarrow r} \left[\omega - \frac{\nabla^2}{2m} \right] A(r r' \omega) \quad (2.33)$$

Again, this is actually $\epsilon(\zeta r)$, and the total energy density is $4\epsilon(r)$.

Our system is now described by the spectral function A and the effective potential V , which are determined as functions of μ by equations (2.18), (2.19), (2.27), and (2.10). The value of μ for free nuclear matter, i.e., for zero pressure, is obtained by solving $\epsilon = \mu \rho$, with ρ and ϵ given by (2.29) and (2.33).

II.2. The Homogeneous Case

In the homogeneous case, A and V depend on the difference of the spatial coordinates, $r - r'$. Therefore, it is useful to introduce their spatial Fourier transforms:

$$A(r r' \omega) = \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot (r - r')} A(p \omega) \quad (2.34)$$

and

$$V(\mathbf{r}\mathbf{r}') = \int \frac{(d\mathbf{p})}{(2\pi)^3} e^{i\mathbf{p}\cdot(\mathbf{r} - \mathbf{r}')} V(\mathbf{p}) \quad . \quad (2.35)$$

In terms of these transforms, (2.18) becomes

$$\left[\omega - \frac{\mathbf{p}^2}{2m} - V(\mathbf{p}) \right] A(\mathbf{p}\omega) = 0 \quad , \quad (2.36)$$

(2.19) becomes

$$\int \frac{d\omega}{2\pi} A(\mathbf{p}\omega) = 1 \quad , \quad (2.37)$$

and (2.27) becomes

$$V(\mathbf{p}) = \int \frac{(d\mathbf{p}')}{(2\pi)^3} \left[v(\mathbf{p}=0) - v_{\text{ex}}(\mathbf{p} - \mathbf{p}') \right] \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(\mathbf{p}'\omega) \quad , \quad (2.38)$$

where $v(\mathbf{p})$ and $v_{\text{ex}}(\mathbf{p})$ are the transforms of the interparticle potentials:

$$v(\mathbf{r}) = \int \frac{(d\mathbf{p})}{(2\pi)^3} e^{i\mathbf{p}\cdot\mathbf{r}} v(\mathbf{p}) \quad (\text{similarly for } v_{\text{ex}}) \quad . \quad (2.39)$$

Now, (2.36) and (2.37) have the solution

$$A(\mathbf{p}\omega) = 2\pi\delta[\omega - h(\mathbf{p})] \quad , \quad (2.40)$$

where

$$h(\mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{p}) \quad . \quad (2.41)$$

By substituting this result into (2.38), we obtain

$$V(\mathbf{p}) = \int_{\Gamma} \frac{(d\mathbf{p}')}{(2\pi)^3} [v(0) - v_{\text{ex}}(\mathbf{p} - \mathbf{p}')] \quad , \quad (2.42)$$

where Γ is the region of momentum space where $\mu - h(\mathbf{p}) > 0$, i.e., the Fermi region. It is simplest to assume that Γ is a sphere, and we will find that this assumption leads to consistent solutions. Let p_f be the radius of this sphere, i.e., the Fermi momentum. Then, (2.42) becomes

$$V(\mathbf{p}) = \frac{v(0)p_f^3}{6\pi^2} - \int_{|\mathbf{p}'| < p_f} \frac{(d\mathbf{p}')}{(2\pi)^3} v_{\text{ex}}(\mathbf{p} - \mathbf{p}') \quad . \quad (2.43)$$

The value of p_f is determined by the relation $\mu - h(p) = 0$ on the surface of Γ , i.e.,

$$\mu = h(p_f) = \frac{p_f^2}{2m} + V(p_f) = \frac{p_f^2}{2m} + \frac{v(0)p_f^3}{6\pi^2} - \int_{|p'| < p_f} \frac{(dp')}{(2\pi)^3} v_{\text{ex}}(p_f - p') \quad (2.44)$$

At this point we may infer the conditions which are necessary to give saturation in the Hartree-Fock approximation. Saturation will occur only if the limit of μ , as $\rho \rightarrow \infty$ or equivalently as $p_f \rightarrow \infty$ is larger or equal to zero. From (2.44) we can see that this will occur if and only if

$$v(p=0) = \int (dr) v(r) \geq 0 \quad , \quad (2.45)$$

i.e., the nonexchange portion of the interparticle potential must be repulsive. Of course, in order for the system to be bound at all, the exchange portion of the potential must be sufficiently attractive to compensate for this repulsion and give a negative value to μ at the saturation density. Our choice of signs is such that v_{ex} must be positive to give such an attraction.

We see here that the Hartree-Fock approximation cannot account for saturation by means of a repulsive core, but must rely upon an exchange effect. Except for the exchange term, the effective potential depends only on a single characteristic of the interparticle potential, the integral $\int (dr) v(r)$, so that if the exchange term were negligible, we would face the dilemma that this quantity should be negative to give binding but positive to give saturation.

The actual value of μ for free nuclear matter is determined by the requirement that the pressure be zero, which leads to the relation $\epsilon = \mu \rho$. To obtain expressions for the particle and energy densities ρ and ϵ , we use (2.34), (2.35), and (2.40) to rewrite (2.29) as

$$\rho = \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} = \frac{p_f^3}{6\pi^2} \quad , \quad (2.46)$$

and (2.33) as

$$\begin{aligned}
\epsilon &= \frac{1}{2} \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \left[h(p) + \frac{p^2}{2m} \right] = \frac{p_f^5}{20\pi^2 m} + \frac{1}{2} \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} V(p) \\
&= \frac{p_f^5}{20\pi^2 m} + \frac{1}{2} \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \int_{|p'| < p_f} \frac{(dp')}{(2\pi)^3} \left[v(0) - v_{ex}(p - p') \right] \quad (2.47)
\end{aligned}$$

Substituting (2.46) and (2.47) into $\epsilon = \mu\rho$, we obtain

$$\mu \frac{p_f^3}{6\pi^2} = \frac{p_f^5}{20\pi^2 m} + \frac{1}{2} v(0) \frac{p_f^6}{36\pi^4} - \frac{1}{2} \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \int_{|p'| < p_f} \frac{(dp')}{(2\pi)^3} v_{ex}(p - p') \quad ; \quad (2.48)$$

equations (2.44) and (2.48) are simultaneous equations determining μ and p_f . Once p_f has been determined, the effective potential is given by (2.43), and the function A by (2.40) and (2.41).

The solution of these equations has been carried out for a case where v and v_{ex} are Gaussian potentials with the same range:

$$\left\{ \begin{array}{l} v(r) \\ v_{ex}(r) \end{array} \right\} = - \left\{ \begin{array}{l} \lambda \\ \lambda_{ex} \end{array} \right\} e^{-\alpha^2 r^2} \quad ; \quad \left\{ \begin{array}{l} v(p) \\ v_{ex}(p) \end{array} \right\} = - \frac{\pi^{3/2}}{\alpha^3} \left\{ \begin{array}{l} \lambda \\ \lambda_{ex} \end{array} \right\} e^{-\frac{p^2}{4\alpha^2}} \quad (2.49)$$

The choice of Gaussian functions was made in order to simplify certain integrations appearing in the inhomogeneous case. In any event, one would not expect the result to be very sensitive to the choice of potential shape.

Using (2.44), (2.48), and (2.49), we obtain an equation for the variable $u = p_f/\alpha$,

$$\frac{\alpha^2 \sqrt{\pi}}{30m} u^5 - \frac{\lambda}{72} u^6 - \frac{\lambda_{ex}}{6} \left[1 - e^{-u^2} - \frac{1}{2} u^2 - \frac{1}{2} u^2 e^{-u^2} \right] = 0 \quad (2.50)$$

The value of the chemical potential is determined by

$$\mu = \frac{p_f^2}{2m} - \frac{\lambda u^3}{6\sqrt{\pi}} - \frac{\lambda_{ex}}{u\sqrt{\pi}} [1 - e^{-u^2}] + \frac{\lambda_{ex}}{2} \operatorname{erf}(u) \quad , \quad (2.51)$$

where

$$\text{erf}(u) = \frac{2}{\sqrt{\pi}} \int_0^u e^{-t^2} dt \quad (2.52)$$

is the conventional definition of the error function. Finally, equation (2.43) for the effective potential becomes

$$V(p) = -\frac{\pi^{3/2}}{\alpha^3} \lambda \frac{P_f^3}{6\pi^2} - \frac{\alpha}{\sqrt{\pi} p} \lambda_{\text{ex}} \left[e^{-\left(\frac{P_f - p}{2\alpha}\right)^2} - e^{-\left(\frac{P_f + p}{2\alpha}\right)^2} \right] \\ + \frac{1}{2} \lambda_{\text{ex}} \left[\text{erf} \frac{P_f + p}{2\alpha} + \text{erf} \frac{P_f - p}{2\alpha} \right] \quad (2.53)$$

The parameters λ , λ_{ex} , and α appearing in (2.49) may be determined by fitting the interparticle potentials to low-energy two-nucleon scattering data and the ground state of the deuteron. Feshbach and Loman⁽⁶⁾ give the following values for the scattering length and effective range for triplet and singlet scattering:

$$\begin{aligned} a_t &= 5.39 \pm 0.03 \text{ fermis} \\ r_t &= 1.703 \pm 0.03 \text{ fermis} \\ a_s &= -23.7 \pm 0.1 \text{ fermis} \\ r_s &= 2.7 \pm 0.5 \text{ fermis} \end{aligned} \quad (2.54)$$

Blatt and Jackson⁽⁷⁾ have computed a set of formulas and graphs for fitting the depth and range of various potential functions to values of a and r . Normally, the quantities in (2.54) would determine four independent parameters, the depth and range of the triplet and singlet potentials. However, the experimental deviation of r_s is sufficiently great that it is possible to set the triplet and singlet potential ranges equal and still fit the data in (2.54) to within the stated accuracy. When this simplifying assumption is made, the application of Blatt and Jackson's fitting procedure, using a Gaussian potential, gives

$$v = v_t P^t + v_s P^s = - [\lambda_t P^t + \lambda_s P^s] e^{-\alpha^2 r^2} \quad (2.55)$$

where

$$\begin{aligned} \alpha &= 0.669 \text{ fermi}^{-1} ; \\ \lambda_t &= 70.67 \text{ Mev} ; \\ \lambda_s &= 46.29 \text{ Mev} , \end{aligned} \quad (2.56)$$

and P^t and P^s are the projection operators for the triplet and singlet spin states:

$$P^t = \frac{1}{2} (1 + P^\sigma) \quad ; \quad P^s = \frac{1}{2} (1 - P^\sigma) \quad . \quad (2.57)$$

The interparticle potential is still not completely determined, however. The data in (2.54) describe S-wave scattering, and therefore will still be fitted correctly if (2.55) is multiplied by the space-exchange operator P_{ex} . More generally, we can replace (2.55) by

$$v = [v_t P^t + v_s P^s] [1 - \eta + \eta P_{ex}] \quad , \quad (2.58)$$

where η is an arbitrary constant. Thus, we have the option of specifying an arbitrary admixture of space exchange in the interparticle potential.

For Fermi-Dirac statistics, the three exchange operators satisfy $P_{ex} = -P^\sigma P^T$. The substitution of this relation and (2.57) into (2.58) gives

$$v = \left[\frac{v_t + v_s}{2} + \frac{v_t - v_s}{2} P^\sigma \right] \left[1 - \eta - \eta P^\sigma P^T \right] \quad . \quad (2.59)$$

The spin-exchange operator satisfies $P^{\sigma 2} = 1$. If we use this relation to expand (2.59) and compare the result with (2.7) and (2.10), we obtain

$$\begin{aligned} v &= 3v_t + v_s - \frac{9}{2} \eta v_t - \frac{1}{2} \eta v_s \quad , \\ v_{ex} &= \frac{3}{2} v_t - \frac{1}{2} v_s - \frac{9}{2} \eta v_t - \frac{1}{2} \eta v_s \quad , \end{aligned} \quad (2.60)$$

where both v_t and v_s are attractive.

Now our choice of η is restricted by the requirement that $v \geq 0$ in order to give saturation. This leads to

$$\eta \geq \eta_0 = \frac{6v_t + 2v_s}{9v_t + v_s} \quad . \quad (2.61)$$

By substituting the values of (2.56), we obtain $\eta_0 = 0.757$.

Two values of η are of special interest: (i) $\eta = \eta_0$, which gives the minimum amount of space exchange necessary to produce saturation; and (ii) $\eta = 1$, which gives a pure space-exchange potential. For these cases, the parameters in (2.49) are

Case (i):

$$\lambda = 0$$

$$\lambda_{ex} = -175.44 \text{ Mev}$$

$$\alpha = 0.669 \text{ fermi}^{-1}$$

Case (ii):

$$\lambda = -82.86 \text{ Mev}$$

$$\lambda_{ex} = -258.30 \text{ Mev}$$

$$\alpha = 0.669 \text{ fermi}^{-1} \quad . \quad (2.62)$$

The remaining parameter in our equations is the mass. We have been using a system of units in which $\hbar = 1$, and have chosen our independent units as Mev's and fermis. In this system the average nucleon mass is $m = 0.0241141 \pm 0.0000017 \text{ Mev}^{-1} \text{ fermi}^{-2}$, or $1/2m = 20.7347 \pm 0.0015 \text{ Mev-fermi}^2$.

Equation (2.50) was solved numerically to give the Fermi momentum for the two cases in (2.62). This equation has two roots:

$$\begin{array}{ll} \text{Case (i):} & \text{Case (ii):} \\ p_f = \begin{cases} 0.34268 \text{ f}^{-1} \\ 1.2226 \text{ f}^{-1} \end{cases} & p_f = \begin{cases} 0.38833 \text{ f}^{-1} \\ 0.65662 \text{ f}^{-1} \end{cases} \end{array} \quad (2.63)$$

The corresponding values of μ , given by (2.51), are

$$\begin{array}{ll} \text{Case (i):} & \text{Case (ii):} \\ \mu = \begin{cases} 0.4349 \text{ Mev} \\ -3.6284 \text{ Mev} \end{cases} & \mu = \begin{cases} 0.4866 \text{ Mev} \\ 0.2982 \text{ Mev} \end{cases} \end{array} \quad (2.64)$$

In both cases the first root gives a positive value for the binding energy $E/N = \mu$, and this solution can be considered nonphysical. In case (ii), however, even the second root gives a positive binding energy. We must assume, therefore, that a pure exchange force cannot yield a bound system (at least in the Hartree approximation), and that only a limited range of the parameter η leads to a physically acceptable result.

Fortunately, the second root in case (i) yields a bound system. For this case, the effective potential was calculated from (2.53), which gave the results tabulated in Table I and shown in Figure 1. One further quantity of interest is the density; equation (2.29) gives $\rho = 0.03087 \text{ f}^{-3}$ (which must be multiplied by a degeneracy factor of four), which corresponds to an interparticle spacing constant of $r_0 = [3/(16\pi\rho)]^{1/3} = 1.25 \text{ fermi}$. The important results of the calculation are summarized in Table II.

Table I. EFFECTIVE POTENTIAL FOR HOMOGENEOUS NUCLEAR MATTER IN THE HARTREE-FOCK APPROXIMATION

$p \text{ (f}^{-1}\text{)}$	$V(p) \text{ (Mev)}$	$p \text{ (f}^{-1}\text{)}$	$V(p) \text{ (Mev)}$
0	-62.53	1.25	-33.70
0.25	-61.02	1.50	-25.55
0.50	-56.70	1.75	-18.37
0.75	-50.14	2.00	-12.50
1.00	-42.17		

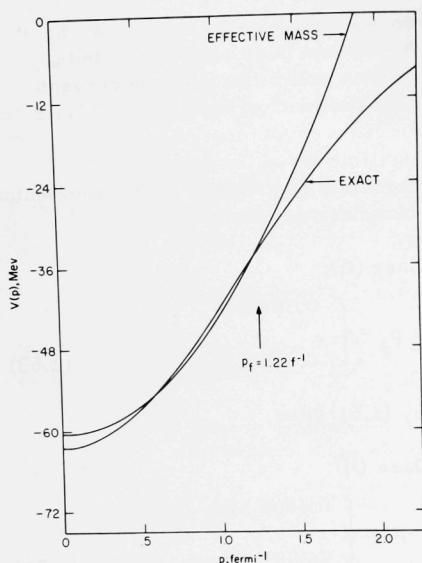


Fig. 1. Effective Potential $V(p)$, as a function of p , for homogeneous nuclear matter in the Hartree-Fock approximation, using the exact and effective-mass solutions.

A comparison of the calculated value of -3.63 Mev with the observed binding energy per particle of -15.75 Mev, obtained from fitting nuclear masses(8) bears out our pessimistic assumptions about the applicability of the Hartree-Fock approximation. On the other hand, the calculated value $r_0 = 1.25$ fermi is in reasonable agreement with the values $r_0 = 1.1$ to 1.2 fermi obtained from high-energy electron scattering data,(9,10) although it is difficult to infer the density of nuclear matter from finite nuclei because of Coulomb repulsion effects. Although one could perhaps improve these results slightly by tinkering with the interparticle-potential shape, it seems reasonable to conclude that exchange-effect saturation will not give a sufficiently large (negative) binding energy. If a repulsive-core saturation mechanism is used, however, Hartree-Fock theory is inapplicable, and we

must include correlation effects in the approximation as in Chapters IV and V.

Table II. PARAMETERS OF HOMOGENEOUS NUCLEAR MATTER IN THE HARTREE-FOCK APPROXIMATION FOR THE EXACT AND EFFECTIVE-MASS SOLUTIONS

	Exact	Eff. Mass
Fermi momentum p_f , (f^{-1})	1.2226	1.2226
Chemical potential μ , (Mev)	-3.628	-3.984
Density ρ^a , (f^{-3})	0.03087	0.03087
Interparticle spacing r_0 , (f)	1.25	1.25
Energy density ϵ^a , (Mev- f^{-3})	-0.1120	-0.1230
Energy per particle ϵ/ρ , (Mev)	-3.628	-3.984
V_0 , (Mev)		-60.437
V_2 , (Mev- f^2)		17.029

^aThese quantities must be multiplied by a degeneracy factor of 4.

II.3. The Effective-mass Approximation

In treating the inhomogeneous case it will be necessary to use an effective-mass approximation. In this approximation the effective potential is approximated by an even quadratic function of momentum. This allows the Schroedinger equation for the one-particle wave functions to be transformed into a local Schroedinger equation with a modified, spatially dependent mass term. In this section we investigate the equivalent approximation in the homogeneous case.

We approximate the effective potential by the function

$$V_{ap}(p) = V_0 + V_2 p^2 \quad . \quad (2.65)$$

To determine the quantities V_0 and V_2 , we fit $V_{ap}(p)$ to $V(p)$ by the criteria of least squares; V_0 and V_2 are chosen to minimize

$$\xi = \int (dp) W(p) [V_{ap}(p) - V(p)]^2 \quad . \quad (2.66)$$

The weight function $W(p)$ must be chosen to give a good fit in the region of momentum up to p_f , but it must go to zero rapidly for larger momenta, since the quadratic function V_{ap} will diverge sharply from V beyond p_f . A suitable choice is the Gaussian function

$$W(p) = e^{-p^2/\beta^2} \quad . \quad (2.67)$$

To determine V_0 and V_2 we substitute (2.65) and (2.67) into (2.66), and then minimize ξ by setting its derivatives with respect to V_0 and V_2 equal to zero. This gives two simultaneous linear equations for V_0 and V_2 , which have the solution

$$\begin{aligned} V_0 &= \frac{1}{\pi^{3/2}} \int (dp) e^{-\frac{p^2}{\beta^2}} \left[\frac{5}{2} \frac{1}{\beta^3} - \frac{p^2}{\beta^5} \right] V(p) \quad , \\ V_2 &= \frac{1}{\pi^{3/2}} \int (dp) e^{-\frac{p^2}{\beta^2}} \left[-\frac{1}{\beta^5} + \frac{2}{3} \frac{p^2}{\beta^7} \right] V(p) \quad , \end{aligned} \quad (2.68)$$

where $V(p)$ is given by (2.43) in general, and by (2.53) for the particular choice of interparticle potentials used in the last section. The substitution of (2.53) leads to

$$V_0 = \frac{-\lambda p_f^3}{6\alpha^3 \sqrt{\pi}} - \frac{2\lambda_{\text{ex}} p_f}{\sqrt{\pi} \sqrt{4\alpha^2 + \beta^2}} \left[1 - \frac{\beta^2 p_f^2}{(4\alpha^2 + \beta^2)^2} \right] e^{-\frac{p_f^2}{4\alpha^2 + \beta^2}} + \lambda_{\text{ex}} \operatorname{erf} \frac{p_f}{\sqrt{4\alpha^2 + \beta^2}},$$

$$V_2 = -\frac{4}{3} \frac{\lambda_{\text{ex}} p_f^3}{\sqrt{\pi} (4\alpha^2 + \beta^2)^{5/2}} e^{-\frac{p_f^2}{4\alpha^2 + \beta^2}}. \quad (2.69)$$

To carry out the effective-mass approximation, we simply replace $V(p)$ by the function $V_{\text{ap}}(p)$ defined by (2.65). Thus, (2.44) is replaced by

$$\mu = V_0 + \left(V_2 + \frac{1}{2m} \right) p_f^2, \quad (2.70)$$

(2.47) becomes

$$\epsilon = \frac{1}{20\pi^2 m} p_f^5 + \frac{1}{12\pi^2} V_0 p_f^3 + \frac{1}{20\pi^2} V_2 p_f^5, \quad (2.71)$$

and $\mu \rho = \epsilon$ becomes

$$\mu \frac{1}{6\pi^2} p_f^3 = \frac{1}{20\pi^2 m} p_f^5 + \frac{1}{12\pi^2} V_0 p_f^3 + \frac{1}{20\pi^2} V_2 p_f^5. \quad (2.72)$$

By substituting (2.70) into (2.72) we may eliminate μ and obtain

$$V_0 = -\left[\frac{2}{5m} + \frac{7}{5} V_2 \right] p_f^2. \quad (2.73)$$

For a particular value of the weight parameter β , the quantities V_0 , V_2 , and p_f are determined by the simultaneous equations (2.69) and (2.73), and μ is then given by (2.70). However, since we have already obtained the exact solution, it is more useful to approach the problem in reverse. We may set p_f equal to its value in the exact case and use (2.69) and (2.73) to determine V_0 , V_2 , and β . This procedure is justified by the fact that $V_{\text{ap}}(p)$ will be a least-squares fit to the exact solution for $V(p)$ only if p_f is the same in the exact and the effective-mass solutions. The resulting value of β is 0.6402 f^{-1} .

This computation was carried out numerically with the same data as in the previous section. The results are summarized in Table II, and the function $V_{\text{ap}}(p)$ is shown in Figure 1 for comparison with the exact $V(p)$.

CHAPTER III

THE HARTREE-FOCK APPROXIMATION IN THE INHOMOGENEOUS CASE

III.1. - The Thomas-Fermi Approximation

Having derived the solution of the homogeneous case in the Hartree-Fock approximation, we now investigate the inhomogeneous case. In this section we describe briefly an approximation, analogous to the Thomas-Fermi model in atomic physics, which may be solved by the Fourier-transform methods used in the previous chapter. Unfortunately, it will appear that this approximation is inapplicable to nuclear matter, at least in the Hartree-Fock case, because of the extreme exchange nature of the forces.

The derivation in Section II.1 applies to both the homogeneous and inhomogeneous cases. The value of μ is taken from the homogeneous calculation, and A and V are determined by the simultaneous integral equations (2.18) and (2.27), along with the normalization condition (2.19) and the interparticle-potential formulas (2.10). However, the restriction of spatial homogeneity is now replaced by the condition that the local properties of the system are functions of one rectilinear coordinate (taken to be the Z -axis), which approach their values for a vacuum in one direction and their values for homogeneous matter in the other. Mathematically, A and V become functions of the average spatial coordinate $\frac{1}{2}(z+z')$ as well as the difference $r-r'$, and they satisfy the boundary conditions

$$A, V \rightarrow \begin{cases} A, V_{\text{vacuum}} & ; \quad \frac{z+z'}{2} \rightarrow -\infty \\ A, V_{\text{homogeneous}} & ; \quad \frac{z+z'}{2} \rightarrow +\infty \end{cases} \quad (3.1)$$

It is useful to introduce the convention of denoting sum and difference coordinates by square brackets:

$$F[R, r] \equiv F\left(R + \frac{r}{2}, R - \frac{r}{2}\right); \quad F(r_1, r_2) \equiv F\left[\frac{r_1+r_2}{2}, r_1-r_2\right] \quad (3.2)$$

Thus, (2.18) may be rewritten as

$$\left[\omega + \frac{1}{2m} \left(\frac{1}{4} \nabla_R^2 + \nabla_R \cdot \nabla_r + \nabla_r^2\right)\right] A[R, \omega] - \int (dr') V\left[R + \frac{r'}{2}, r-r'\right] A\left[R - \frac{r-r'}{2}, r', \omega\right] = 0 \quad (3.3)$$

and (2.27) as

$$V[Rr] = \delta(r) \int (dR') v(R - R') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A[R' 0 \omega] - v_{ex}(r) \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A[Rr\omega] \quad (3.4)$$

In the Thomas-Fermi approximation we assume that A and V are slowly varying functions of the sum coordinate R . Then we may approximate (3.3) by dropping the derivatives with respect to this coordinate and setting all sum coordinates equal to R :

$$\left(\omega + \frac{\nabla_r^2}{2m} \right) A[Rr\omega] - \int (dr') V[R, r - r'] A[Rr'\omega] \cong 0 \quad (3.5)$$

This is an integrodifferential equation in the difference coordinates only. If we introduce the Fourier transforms in these coordinates,

$$A[Rr\omega] = \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot r} A(Rp\omega) \quad (3.6)$$

and

$$V[Rr] = \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot r} V(Rp) \quad (3.7)$$

then $A(Rp\omega)$ is determined by the correctly normalized solution of the transform of (3.5):

$$A(Rp\omega) = 2\pi \delta(\omega - h(Rp)) \quad (3.8)$$

where

$$h(Rp) = (p^2/2m) + V(Rp) \quad (3.9)$$

The transformation of (3.4) in the difference coordinates yields

$$\begin{aligned} V(Rp) = & \int (dR') v(R - R') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \int \frac{(dp')}{(2\pi)^3} A(R'p'\omega) \\ & - \int \frac{(dp')}{(2\pi)^3} v_{ex}(p - p') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(Rp'\omega) \quad (3.10) \end{aligned}$$

where $v_{ex}(p)$ is given by (2.39). As in the infinite case, the substitution of (3.8) reduces (3.10) to

$$V(Rp) = \int (dR') v(R - R') \int_{\Gamma(R')} \frac{(dp')}{(2\pi)^3} - \int_{\Gamma(R)} \frac{(dp')}{(2\pi)^3} v_{\text{ex}}(p - p') \quad , \quad (3.11)$$

where $\Gamma(R)$ is the region of momentum space where $\mu - h(Rp) > 0$.

Our system is restricted to a one-dimensional spatial dependence, i.e., $h(Rp)$, $V(Rp)$, and $\Gamma(R)$ are independent of X and Y . If we define

$$v(Z) = \int dXdY v(R) \quad , \quad (3.12)$$

then (3.11) reduces to

$$V(Zp) = \int dZ' v(Z - Z') \int_{\Gamma(Z')} \frac{(dp')}{(2\pi)^3} - \int_{\Gamma(Z)} \frac{(dp')}{(2\pi)^3} v_{\text{ex}}(p - p') \quad . \quad (3.13)$$

We now let $p_f(Z)$ be some point on the surface of $\Gamma(Z)$. This gives the relation $\mu = h(R, p_f(Z))$, and by substituting (3.9) and (3.13) we may obtain

$$\mu = \frac{p_f^2(Z)}{2m} + \int dZ' v(Z - Z') \int_{\Gamma(Z')} \frac{(dp')}{(2\pi)^3} - \int_{\Gamma(Z)} \frac{(dp')}{(2\pi)^3} v_{\text{ex}}(p_f(Z) - p') \quad . \quad (3.14)$$

(There is a restriction on this equation. It cannot be assumed a priori that the density goes to zero asymptotically as $z \rightarrow -\infty$; instead, there may be regions of the Z -axis for which the density is exactly zero in this approximation. In these regions $\Gamma(Z)$ will be empty and $p_f(Z)$ will not be defined. Equation (3.14) applies, however, to all regions where the density is nonzero.)

At this point the shortcomings of the Thomas-Fermi approximation are fairly apparent. Equation (3.14) must be used to relate quantities at different points along the Z -axis, but such a relationship occurs only through the second term on the right-hand side, which is proportional to the nonexchange interparticle potential. Since this part of the potential must be small and repulsive to give saturation, poor or even inconsistent results can be expected.

Actually, a repulsive nonexchange potential leads to an inconsistency. For a reasonably smooth potential this restriction on the nonexchange potential implies that $v(Z)$ is everywhere non-negative. Then the first two terms of the right-hand side of (3.14) are positive, and we have

$$\int_{\Gamma(Z)} \frac{(dp')}{(2\pi)^3} v_{\text{ex}}(p_f(Z) - p') > -\mu \quad . \quad (3.15)$$

Since $-\mu$ is positive, this equation places a lower limit on the magnitude of the integral, and thus a lower limit on the volume of integration. But this volume is proportional to the density $\rho(Z)$, so that (3.14) has no solutions for which $\rho(Z)$ goes continuously to zero as $Z \rightarrow -\infty$, as required by the spatial boundary conditions (3.1).

This failure gives a certain amount of negative information by casting doubt on the original assumption that A and V are slowly varying functions of Z . Actually, the nuclear surface in the Hartree approximation can be assumed to be quite sharp (as it is experimentally), with a thickness of the order of magnitude of the Fermi wavelength.

III.2. - The Wave-function Expansion Method

We now turn to the possibility of solving the inhomogeneous case by expanding A into a set of one-particle wave functions, as in (2.20) and (2.21). The first step is the conversion of (2.18) into a differential equation for the wave functions and the derivation of the normalization conditions.

Now, in Chapter IV we are going to need an analogous derivation for an equation similar to (2.18) but with an energy-dependent effective potential $V(r, r', \omega)$. [This is equation (4.49).] Because of this we will generalize the present derivation slightly to make the potential dependent upon energy, and then reduce our final equations to the energy-independent case.

Thus, (2.18) may be written in the (generalized) form⁽⁵⁾

$$\left[\omega + \frac{\nabla^2}{2m} \right] A(r, r', \omega) - \int (dr'') V \left[r - \frac{r''}{2}, r'', \omega \right] A(r - r'', r', \omega) = 0 \quad (3.16)$$

By defining an asymmetric Fourier transform of V ,

$$V \left[R - \frac{r}{2}, r, \omega \right] = \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot r} \bar{V}(R, p, \omega) \quad (3.17)$$

we may rewrite (3.16) as

$$\left(\omega + \frac{\nabla^2}{2m} \right) A(r, r', \omega) - \int \frac{(dp)}{(2\pi)^3} \bar{V}(r, p, \omega) \left[\int (dr'') e^{ip \cdot r''} A(r - r'', r', \omega) \right] = 0 \quad (3.18)$$

In the bracketed quantity, $A(r - r'', r', \omega)$ may be expanded in a Taylor series about $A(r, r', \omega)$, and the powers of r'' written as derivatives of the exponential. This gives

$$\int (dr'') e^{ip \cdot r''} A(r - r'', r', \omega) = \sum_{n=0}^{\infty} \frac{1}{n!} \int (dr'') \left[-\frac{1}{i} \nabla_p \cdot \nabla_r \right]^n e^{ip \cdot r''} A(r, r', \omega) \quad (3.19)$$

When this is substituted into (3.18), the derivatives with respect to p may be transferred to act on $\bar{V}(r p \omega)$ by integrating by parts. The r'' -integration then acts only on the exponential, which reduces to $\delta(p)$ and undoes the momentum integration. The result is

$$\left[\omega + \frac{\nabla^2}{2m} \right] A(r r' \omega) - \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{1}{i} \nabla_p \cdot \nabla_r \right]^n \bar{V}(r'' p \omega) A(r r' \omega) \Big|_{\substack{p=0 \\ r''=r}} = 0 \quad (3.20)$$

The sum is just a Taylor expansion of $\bar{V}(r'' p \omega)$ with the powers of p replaced by powers of $1/i \nabla_r$. This is formally equivalent to

$$\left[\omega + \frac{\nabla^2}{2m} \right] A(r r' \omega) - \bar{V}\left(r, \frac{1}{i} \nabla_r, \omega\right) A(r r' \omega) = 0 \quad , \quad (3.21)$$

with the understanding that the derivatives act only on A rather than \bar{V} itself.

The asymmetric transform \bar{V} is related to the symmetric transform defined by (3.7). The substitution of (3.7) into the inverse of (3.17) gives

$$\bar{V}(R p \omega) = \int (dr) \int \frac{(dp')}{(2\pi)^3} e^{-i(p-p') \cdot r} V\left(R - \frac{r}{2}, p', \omega\right) \quad (3.22)$$

As before, $V\left(R - \frac{r}{2}, p', \omega\right)$ may be expanded in a Taylor series about $V(R, p', \omega)$, and the powers of r replaced by derivatives of the exponential. The r -integration then yields a delta function, and (3.22) reduces to

$$\bar{V}(R p \omega) = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\frac{1}{2i} \nabla_p \cdot \nabla_R \right]^n V(R p \omega) \quad (3.23)$$

Because of the one-dimensional spatial variation, $V(R p \omega)$ is independent of X and Y , and $A(r r' \omega)$ depends on these coordinates only through their differences $x - x'$ and $y - y'$. Thus, it is useful to introduce a two-dimensional Fourier transform

$$A(r r' \omega) = \int \frac{dp_x dp_y}{(2\pi)^2} e^{ip_x(x-x') + ip_y(y-y')} A\left(p_x p_y z z' \omega - \frac{p_x^2 + p_y^2}{2m}\right) \quad (3.24)$$

which allows (3.21) to be rewritten as

$$\left[\omega + \frac{1}{2m} \frac{\partial^2}{\partial z^2} \right] A(p_x p_y z z' \omega) - \bar{V} \left(z, p_x p_y \frac{1}{i} \frac{\partial}{\partial z}, \omega + \frac{p_x^2 + p_y^2}{2m} \right) A(p_x p_y z z' \omega) = 0 \quad (3.25)$$

Furthermore, because our system is invariant under rotations in the X,Y-plane, A and \bar{V} depend on p_x and p_y only through the magnitude

$$p_r = \sqrt{p_x^2 + p_y^2} \quad (3.26)$$

The one-dimensional wave equation corresponding to (3.25) is

$$\left[\omega + \frac{1}{2m} \frac{\partial^2}{\partial z^2} - \bar{V} \left(z, p_r, \frac{1}{i} \frac{\partial}{\partial z}, \omega + \frac{p_r^2}{2m} \right) \right] \psi(z, p_r, \omega) = 0 \quad (3.27)$$

Consider the limits of \bar{V} as $z \rightarrow \pm \infty$. Since V approaches a constant value in both limits, all terms in (3.23) except the first vanish. Thus, (3.1) gives

$$\bar{V} \left(z, p_r, \frac{1}{i} \frac{\partial}{\partial z}, \omega + \frac{p_r^2}{2m} \right) \rightarrow \begin{cases} 0 & ; z \rightarrow -\infty \\ V_{\text{homogeneous}} \left(p_r, \frac{1}{i} \frac{\partial}{\partial z}, \omega + \frac{p_r^2}{2m} \right) & ; z \rightarrow +\infty \end{cases} \quad (3.28)$$

As $z \rightarrow +\infty$, the wave function has the limit

$$\psi(z, p_r, \omega) \xrightarrow{z \rightarrow \infty} c \sin[kz + \eta(k)] \quad (3.29)$$

where k satisfies

$$\omega - \frac{k^2}{2m} - V_{\text{hom}} \left(\sqrt{p_r^2 + k^2}, \omega + \frac{p_r^2}{2m} \right) = 0 \quad (3.30)$$

which may be written as

$$\omega + \frac{p_r^2}{2m} = h \left(\sqrt{p_r^2 + k^2} \right) \quad (3.31)$$

where $h(p)$ is the solution of

$$h(p) = \frac{p^2}{2m} + V_{\text{hom}}(p, h(p)) \quad (3.32)$$

[We note that in the Hartree case, where V is energy independent, this reduces to (2.41).]

Now $k = 0$ when $\omega = V_{\text{hom}}(p_r, h(p_r))$, so that (3.27) will have a solution only when $\omega > V_{\text{hom}}(p_r, h(p_r))$. (We assume that \bar{V} is smooth enough that no bound states occur.) In addition, since $\bar{V} \rightarrow 0$ as $z \rightarrow -\infty$, there will be a second independent solution when $\omega > 0$. Thus the wave-function decomposition of A is

$$A(p_r, z, z', \omega) = \begin{cases} 0 & ; \omega < V_{\text{hom}}(p_r, h(p_r)) \\ \psi(z, p_r, \omega) \psi^*(z', p_r, \omega) & ; V_{\text{hom}}(p_r, h(p_r)) < \omega < 0 \\ \psi_1(z, p_r, \omega) \psi_1^*(z', p_r, \omega) + \psi_2(z, p_r, \omega) \psi_2^*(z', p_r, \omega) & ; \omega > 0 \end{cases} \quad (3.33)$$

We will need to find the wave functions only in the middle region $V_{\text{hom}}(p_r, h(p_r)) < \omega < 0$, and will limit our attention to this region.

To determine the normalization conditions we use (3.1) to connect the limit of A as $z, z' \rightarrow +\infty$ with the function A which was obtained in the homogeneous case. We assume that the homogeneous A is

$$A_{\text{hom}}(p, \omega) = 2\pi \rho(p) \delta(\omega - h(p)) \quad , \quad (3.34)$$

where

$$\rho(p) = \left[1 - \frac{\partial}{\partial \omega} V_{\text{hom}}(p, h(p)) \right]^{-1} \quad . \quad (3.35)$$

[In the Hartree approximation $\rho(p) = 1$, and (3.34) reduces to (2.40).] Application of (2.34) and (3.24) gives the two-dimensional transform

$$A_{\text{hom}}(p_r, z, z', \omega) = \int dp_z e^{ip_z(z-z')} \rho(p) \delta\left(\omega + \frac{p_r^2}{2m} - h(p)\right) \Big|_{p=\sqrt{p_r^2+p_z^2}} \quad (3.36)$$

From (3.32) we may obtain the derivative

$$\frac{d}{dp} h(p) = \rho(p) \left[\frac{p}{m} + \frac{\partial}{\partial p} V_{\text{hom}}(p, h(p)) \right] \quad , \quad (3.37)$$

which reduces (3.36) to

$$\begin{aligned} A_{\text{hom}}(p_r, z, z', \omega) &= \frac{e^{ik(z-z')} + e^{-ik(z-z')}}{2k \left[\frac{1}{2m} + \frac{1}{2p} \frac{\partial}{\partial p} V_{\text{hom}}(p, h(p)) \right]} \\ &= \frac{\cos k(z-z')}{k \left[\frac{1}{2m} + \frac{1}{2p} \frac{\partial}{\partial p} V_{\text{hom}}(p, h(p)) \right]} \quad , \quad (3.38) \end{aligned}$$

where k is determined by (3.30) or equivalently (3.31) and (3.32).

On the other hand, the substitution of (3.29) into (3.33) yields

$$A(p_r z z' \omega) \xrightarrow{z, z' \rightarrow \infty} \frac{|c|^2}{2} \{ \cos k(z - z') - \cos [k(z + z') + 2\eta(k)] \} \quad (3.39)$$

The second cosine term may be neglected, since it becomes rapidly oscillating for large z and z' , and will vanish in any integration over k . Comparison of the remainder of (3.39) with (3.38) establishes the normalization

$$c = \left\{ \frac{2}{k \left[\frac{1}{2m} + \frac{1}{2p} \frac{\partial}{\partial p} V_{\text{hom}}(p, h(p)) \right]} \right\}^{1/2}, \quad (3.40)$$

where the phase has been chosen to yield real wave functions.

Even for numerical calculation, (3.27) will be reasonably tractable only if the effective potential has a simple momentum dependence. Therefore, in the following derivations we use a generalized effective-mass approximation similar to that in Section II.3, in which this dependence is assumed to be even and quadratic. However, V cannot be assumed a priori to be independent of the direction of p , but only of the orientation in the p_x, p_y -plane. We must use the form

$$V(z p \bar{\omega}) = V_0(z \bar{\omega}) + V_{\perp}(z \bar{\omega}) p_r^2 + V_{\parallel}(z \bar{\omega}) p_z^2, \quad (3.41)$$

where $\bar{\omega} = \omega + (p_r^2/2m)$. Equation (3.23) then gives

$$\begin{aligned} \bar{V}(z p \bar{\omega}) = & V_0(z \bar{\omega}) + V_{\perp}(z \bar{\omega}) p_r^2 \\ & - \frac{1}{4} \frac{d^2}{dz^2} V_{\parallel}(z \bar{\omega}) + \frac{1}{i} \frac{d}{dz} V_{\parallel}(z \bar{\omega}) p_z + V_{\parallel}(z \bar{\omega}) p_z^2 \end{aligned} \quad (3.42)$$

By substituting this into (3.27) we obtain

$$\begin{aligned} \frac{\partial}{\partial z} \left[\left(V_{\parallel}(z \bar{\omega}) + \frac{1}{2m} \right) \frac{\partial}{\partial z} \psi(z p_r \omega) \right] = \\ \left[-\omega + V_0(z \bar{\omega}) + V_{\perp}(z \bar{\omega}) p_r^2 - \frac{1}{4} \frac{d^2}{dz^2} V_{\parallel}(z \bar{\omega}) \right] \psi(z p_r \omega) \end{aligned} \quad (3.43)$$

This is a local Schroedinger equation in which the mass has been replaced by a spatially dependent function. To remove this dependence we make the substitution

$$\psi(z p_r \omega) = \left[V_{||}(z \bar{\omega}) + \frac{1}{2m} \right]^{-1/2} \phi(z p_r \omega) \quad , \quad (3.44)$$

which reduces (3.43) to

$$\frac{\partial^2}{\partial z^2} \phi(z p_r \omega) = \left\{ \frac{-\omega + V_0(z \bar{\omega}) + V_{\perp}(z \bar{\omega}) p_r^2}{V_{||}(z \bar{\omega}) + \frac{1}{2m}} + \frac{1}{4} \frac{d}{dz} \left(\frac{\frac{d}{dz} V_{||}(z \bar{\omega})}{V_{||}(z \bar{\omega}) + \frac{1}{2m}} \right) \right\} \phi(z p_r \omega) \quad . \quad (3.45)$$

In establishing the normalization we must use the homogeneous effective potential of Section II.3, which was derived using the effective-mass approximation. With our generalized energy dependence this has the form

$$V_{\text{hom}}(p \bar{\omega}) = V_{0 \text{ hom}}(\bar{\omega}) + V_{2 \text{ hom}}(\bar{\omega}) p^2 \quad . \quad (3.46)$$

Therefore, in the limit $z \rightarrow +\infty$,

$$\begin{aligned} V_0(z \bar{\omega}) &\rightarrow V_{0 \text{ hom}}(\bar{\omega}) \quad , \\ V_{\perp}(z \bar{\omega}) &\rightarrow V_{2 \text{ hom}}(\bar{\omega}) \quad , \\ V_{||}(z \bar{\omega}) &\rightarrow V_{2 \text{ hom}}(\bar{\omega}) \quad . \end{aligned} \quad (3.47)$$

The substitution of (3.46) into (3.40) gives

$$c = \left\{ \frac{2}{k \left[V_{2 \text{ hom}}(\bar{\omega}) + \frac{1}{2m} \right]} \right\}^{1/2} \quad . \quad (3.48)$$

If we substitute this into (3.29) and compare the result with (3.44), we obtain the normalization condition

$$\phi(z p_r \omega) \xrightarrow{z \rightarrow \infty} \sqrt{2/k} \sin [kz + \eta(k)] \quad . \quad (3.49)$$

The simple momentum dependence of (3.46) allows us to solve (3.30) explicitly for k , obtaining

$$k = \left\{ \frac{\omega - V_{0 \text{ hom}}(\bar{\omega}) - V_{2 \text{ hom}}(\bar{\omega}) p_r^2}{V_{2 \text{ hom}}(\bar{\omega}) + \frac{1}{2m}} \right\}^{1/2} \quad . \quad (3.50)$$

In summary, we have defined a partially transformed spectral function $A(p_r z z' \omega)$ by (3.24) and expressed this function as a product of wave functions in (3.33). In the effective-mass approximation these wave functions satisfy (3.44) and (3.45), with the normalization being determined by (3.49) and (3.50).

We must now obtain expressions for the density and effective potential in terms of the partially transformed A . At this point we discard the generalization of an energy-dependent effective potential and again limit our derivation to the Hartree-Fock case. To find the density we substitute (3.24) into (2.29) and rewrite the p_x, p_y -integration in polar coordinates, obtaining

$$\rho(z) = \int_0^{P_f} \frac{p_r dp_r}{2\pi} \int_{V_{0\text{hom}} + V_{2\text{hom}} p_r^2}^{\mu - (p_r^2/2m)} \frac{d\omega}{2\pi} A(p_r z z' \omega) \quad (3.51)$$

The finite area of integration in (3.51) is caused by the lower bound of the energy spectrum of the wave functions, given by (3.33). This establishes a lower limit to the ω -integration, and truncates the p_r -integration at p_f , for which the ω -limits are equal.

Similarly, to find the effective potential we substitute (3.24) and (2.29) into (2.27), and transform the resulting expression according to (3.27). This gives

$$\begin{aligned} V(Z p_r p_Z) = & \int dZ' v(Z - Z') \rho(Z') - Z \int_0^{P_f} \frac{p_r' dp_r'}{2\pi} \int_{V_{0\text{hom}} + V_{2\text{hom}} p_r'^2}^{\mu - (p_r'^2/2m)} \frac{d\omega}{2\pi} \int_0^\infty dz \\ & \times \left[\int_0^{2\pi} \frac{d\theta}{2\pi} \int_{-\infty}^\infty \frac{dp_Z'}{2\pi} \cos p_Z' z v_{\text{ex}} \left(\sqrt{p_r^2 - 2 p_r p_r' \cos \theta + p_r'^2 + (p_Z - p_Z')^2} \right) \right] \\ & A\left(p_r', Z + \frac{z}{2}, Z - \frac{z}{2}, \omega\right) \quad , \end{aligned} \quad (3.52)$$

where $v(Z)$ is defined by (3.12) and $v_{\text{ex}}(p)$ by (2.39). If v and v_{ex} are the Gaussian potentials (2.49), this reduces to

$$\begin{aligned} V(Z p_r p_Z) = & - \frac{\pi \lambda}{\alpha^2} \int_{-\infty}^\infty dZ' e^{-\alpha^2(Z - Z')^2} \rho(Z') + \frac{2\pi \lambda_{\text{ex}}}{\alpha^2} \int_0^{P_f} \frac{p_r' dp_r'}{2\pi} e^{-\frac{p_r^2 + p_r'^2}{4\alpha^2}} I_0 \left(\frac{p_r p_r'}{2\alpha^2} \right) \\ & \times \int_{V_{0\text{hom}} + V_{2\text{hom}} p_r'^2}^{\mu - (p_r'^2/2m)} \frac{d\omega}{2\pi} \int_0^\infty dz e^{-\alpha^2 z^2} \cos p_Z z A\left(p_r', Z + \frac{z}{2}, Z - \frac{z}{2}, \omega\right) \quad , \end{aligned} \quad (3.53)$$

where I_0 is the imaginary Bessel function of the first kind.

To carry out the effective-mass approximation we must approximate (3.53) by a quadratic function of the form (3.41). This is done by the least-squares procedure of Section II.3; the quantity

$$\xi(z) = \int (dp) e^{-(p^2/\beta^2)} [V_0(z) + V_{\perp}(z) p_r^2 + V_{\parallel}(z) p_z^2 - V(z)p]^2 \quad (3.54)$$

is minimized by setting its derivatives with respect to V_0 , V_{\perp} , and V_{\parallel} equal to zero. The solution of the resulting simultaneous equations is

$$V_i(Z) = \sum_j M_{ij} U_j(Z) \quad , \quad (3.55)$$

where

$$U_j(Z) = \frac{1}{\beta^3 \pi^{3/2}} \int (dp) e^{-(p^2/\beta^2)} \left\{ \begin{matrix} 1 \\ p_r^2 \\ p_z^2 \end{matrix} \right\} V(Z, p) \quad , \quad (3.56)$$

and

$$M = \begin{matrix} & \begin{matrix} 0 & \perp & \parallel \end{matrix} \\ \begin{matrix} 0 \\ \perp \\ \parallel \end{matrix} & \begin{bmatrix} \frac{5}{2} & -\frac{1}{\beta^2} & -\frac{1}{\beta^2} \\ -\frac{1}{\beta^2} & \frac{1}{\beta^4} & 0 \\ -\frac{1}{\beta^2} & 0 & \frac{2}{\beta^4} \end{bmatrix} \end{matrix} \quad . \quad (3.57)$$

Combining (3.55) to (3.57) with (3.53) gives

$$\left\{ \begin{matrix} 0 \\ \perp \\ \parallel \end{matrix} \right\} (Z) = \left\{ \begin{matrix} -\frac{\lambda \pi}{\alpha^2} \int_{-\infty}^{\infty} dZ' e^{-\alpha^2(Z-Z')^2} \rho(Z') \\ 0 \\ 0 \end{matrix} \right\} \\ + \frac{8\pi\lambda \text{ex}}{4\alpha^2 + \beta^2} \int_0^{P_f} \frac{p_r dp_r}{2\pi} \int_{V_{0\text{hom}} + V_{2\text{hom}} p_r^2}^{\mu - (p_r^2/2m)} \frac{d\omega}{2\pi} e^{-\frac{p_r^2}{4\alpha^2 + \beta^2}} \\ \left\{ \begin{bmatrix} \left(2 - \frac{4\alpha^2}{4\alpha^2 + \beta^2} - \frac{\beta^2 p_r^2}{(4\alpha^2 + \beta^2)^2} \right) \mathcal{L}_0 + \frac{\beta^2}{4} \mathcal{L}_z \\ \left(-\frac{1}{4\alpha^2 + \beta^2} + \frac{p_r^2}{(4\alpha^2 + \beta^2)^2} \right) \mathcal{L}_0 \\ \left(-\frac{1}{2} \right) \mathcal{L}_z \end{bmatrix} \right\} \quad (3.58)$$

where

$$J_{\left\{ \begin{smallmatrix} 0 \\ 2 \end{smallmatrix} \right\}}(Z p_r \omega) = \int_0^{\infty} dz e^{-(\alpha^2 + \frac{1}{4} \beta^2) z^2} \left\{ \begin{smallmatrix} 1 \\ z^2 \end{smallmatrix} \right\} A(p_r, Z + \frac{z}{2}, Z - \frac{z}{2}, \omega) \quad (3.59)$$

In the near-vacuum region it is possible to make a conjecture as to an analytic approximation to the potentials. In this region the semi-bound wave functions will be approximately proportional to $\exp(\sqrt{-2m\omega} z)$. The slowest decaying wave function, which presumably will dominate the integrals in (3.58), occurs for $\omega = \mu$. Thus, we may expect that, as $z \rightarrow -\infty$, V_0 , V_{\perp} , and V_{\parallel} will go to zero as the square of this function, i.e., as $\exp(2\sqrt{-2m\mu} z)$.

III.3. Numerical Computation

At this point the main problem is the solution of the Schroedinger equation (3.45). A perturbation method seems feasible, but, unfortunately, if we require the unperturbed potential to approach zero on one side and $V_0 + V_2 p_r^2$ on the other, the simplest possible unperturbed wave functions are hypergeometric functions, and the resulting integrals are completely intractable. It seems preferable to treat the equation by direct point-by-point numerical integration. By using such a method, the solution of the inhomogeneous case can be determined by an iterative procedure in which during each iteration the semi-bound wave functions are calculated for an approximate effective potential, and then a closer approximation to the effective potential is obtained by integrating the wave functions.

Such a computation was programmed for an IBM 704 Electronic Data Processing Machine. During each iteration the computer begins with a table of the functions $V_0(z)$, $V_{\perp}(z)$, and $V_{\parallel}(z)$ covering a z -range of 8 fermis, and performs the following calculations:

- 1) The table of $V_0(z)$, $V_{\perp}(z)$, and $V_{\parallel}(z)$ is extended on each side by about $2\frac{1}{2}$ fermis. In the right-hand region these functions are set equal to their values for the homogeneous case. On the left, they are extended by assuming that they are proportional to $\exp(2\sqrt{-2m\mu} z)$.
- 2) The various derivatives and products of V_0 , V_{\perp} , and V_{\parallel} which appear in (3.45) are calculated.
- 3) For given values of p_r and ω , a table of the wave function $\phi(z p_r \omega)$ is calculated in the left-hand extension by assuming that the potential term in (3.45) is proportional to $\exp(2\sqrt{-2m\mu} z)$. Such a potential has wave functions which are Bessel functions, of the first kind and nonintegral order, of an exponential of z .

4) The table of $\phi(z p_r \omega)$ is computed for the remaining z -range by point-by-point solution of (3.45). A modification of Noumerov's method is used which gives an error at each point of the order of the eighth power of the mesh spacing.

5) The normalizing constant is computed from the values of the wave function and its derivative at the midpoint of the right-hand extension. The entire wave function is multiplied by a constant to give a normalization satisfying (3.49), and (3.44) is used to transform the wave function into $\psi(z p_r \omega)$.

6) The integrals \mathcal{J}_0 and \mathcal{J}_2 in (3.59) are calculated for the non-extended z -range of 8 fermis.

7) Steps 3) to 6) are repeated for various values of p_r and ω covering the region of integration in (3.58). A new table of $V_0(z)$, $V_{\perp}(z)$, and $V_{\parallel}(z)$ is built up by integrating \mathcal{J}_0 and \mathcal{J}_2 over these variables. In the same manner, (3.51) is used to compute the density $\rho(z)$.

The computation was performed with the use of the parameters obtained in the solution of the homogeneous case by the effective-mass approximation, i.e., the data in Table II. The initial table of the V 's was obtained from the formula

$$\left. \begin{array}{l} V_0(z) \\ V_{\perp}(z) \\ V_{\parallel}(z) \end{array} \right\} \cong \frac{e^{1.5(z-3.5)}}{1 + e^{1.5(z-3.5)}} \left\{ \begin{array}{l} V_0 \text{ hom} \\ V_2 \text{ hom} \\ V_2 \text{ hom} \end{array} \right. \quad (3.60)$$

Nineteen iterations were carried out. The early iterations, which used a mesh spacing of $\frac{1}{8}$ fermi and a 12-point formula for the p_r and ω integrations, required $4\frac{1}{3}$ min apiece. During later iterations the mesh spacing was halved and a 16-point integration formula was used. On the last iteration (3.52) was used to compute a table of $V(z p_r p_z)$ from the approximate wave functions. The entire computation required about 2 hr.

The density and potential functions obtained from the last iteration are tabulated in Table III and are shown in Figures 2 and 3. The surface is seen to be quite sharp, as expected, with an exponential tail on the vacuum side and a strongly damped oscillation on the interior side which is apparently due to the formation of standing waves. The functions $V_{\perp}(z)$ and $V_{\parallel}(z)$ are nearly equal, although there is no obvious theoretical reason for this. Figure 4 gives a set of momentum profiles of $V(z p_r p_z)$ for various points along the Z -axis.

Table III

DENSITY AND EFFECTIVE POTENTIAL ACROSS A PLANE
SURFACE OF NUCLEAR MATTER, IN THE
HARTREE-FOCK APPROXIMATION

Z (f)	$\rho^a (\text{f}^{-3})$	V_0 (Mev)	V_{\perp} (Mev-f ²)	V_{\parallel} (Mev-f ²)
0.0	0.0003934	-1.175	0.3847	0.4669
0.25	0.0004214	-1.292	0.4207	0.5281
0.50	0.0004808	-1.471	0.4767	0.6081
0.75	0.0005820	-1.742	0.5624	0.7134
1.00	0.0007426	-2.152	0.6920	0.8576
1.25	0.0009912	-2.768	0.8861	1.063
1.50	0.001371	-3.689	1.174	1.361
1.75	0.001948	-5.050	1.597	1.793
2.00	0.002809	-7.033	2.208	2.407
2.25	0.004070	-9.854	3.070	3.261
2.50	0.005856	-13.74	4.247	4.412
2.75	0.008275	-18.87	5.786	5.900
3.00	0.01136	-25.29	7.689	7.734
3.25	0.01505	-32.79	9.889	9.862
3.50	0.01909	-40.92	12.23	12.16
3.75	0.02317	-48.95	14.50	14.43
4.00	0.02687	-56.06	16.46	16.43
4.25	0.02987	-61.53	17.89	17.94
4.50	0.03192	-64.88	18.68	18.80
4.75	0.03296	-66.05	18.83	18.99
5.00	0.03308	-65.35	18.46	18.63
5.25	0.03252	-63.45	17.79	17.94
5.50	0.03162	-61.16	17.06	17.17
5.75	0.03072	-59.21	16.49	16.56
6.00	0.03009	-58.08	16.21	16.23
6.25	0.02985	-57.92	16.23	16.21
6.50	0.02997	-58.52	16.48	16.43
6.75	0.03032	-59.55	16.83	16.78
7.00	0.03074	-60.58	17.15	17.11
7.25	0.03110	-61.32	17.36	17.34
7.50	0.03131	-61.63	17.42	17.43
7.75	0.03137	-61.53	17.35	17.37
8.00	0.03127	-61.17	17.21	17.23
∞	0.03087	-60.44	17.03	17.03

^aThese quantities must be multiplied by a degeneracy factor of 4.

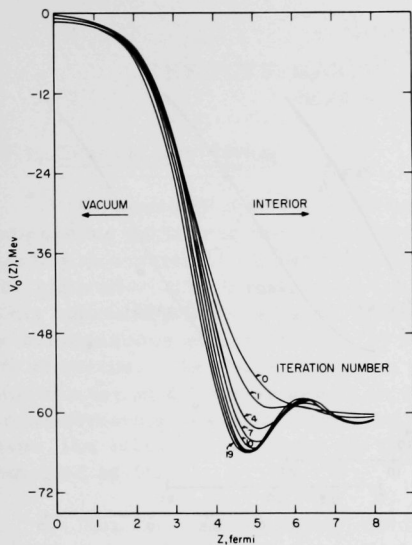
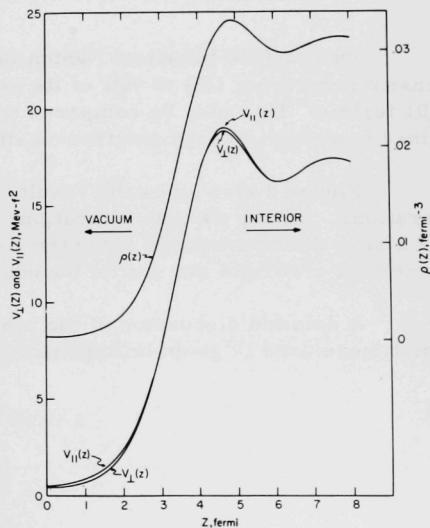


Fig. 2

The momentum-independent term $V_0(z)$ of the effective-mass approximation for the effective potential across a plane surface of nuclear matter, in the Hartree-Fock approximation. The quantity is given as a function of z and is shown after each iteration of the self-consistent computation.

Fig. 3

The density $\rho(z)$ and the quadratic terms $V_{\perp}(z)$ and $V_{\parallel}(z)$ of the effective-mass approximation for the effective potential across a plane surface of nuclear matter, in the Hartree-Fock approximation. All quantities are given as functions of z . The two terms V_{\perp} and V_{\parallel} , which are coefficients of the momentum components perpendicular and parallel to the z axis, are equal within the limited accuracy of the graph, except in the shoulder regions where a small difference is indicated by splitting the curves. The density $\rho(z)$ must be multiplied by a degeneracy factor of 4.



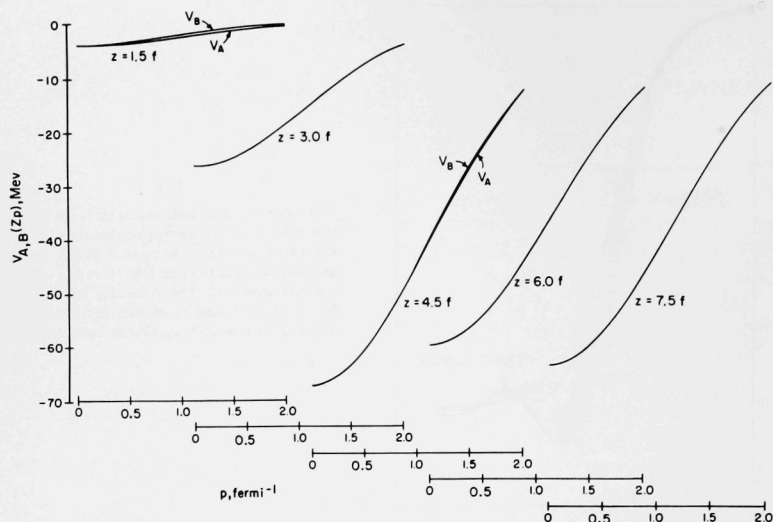


Fig. 4. The effective potential $V(z, p)$ across a plane surface of nuclear matter in the Hartree-Fock approximation. In this case, $V(z, p)$ was computed without the effective-mass approximation [i.e., from Eq. (3.52)] but from wave functions which were obtained with the effective-mass approximation. Two functions $V_A(z, p) = V(z, p_r = p, p_z = 0)$ and $V_B(z, p) = V(z, p_r = 0, p_z = p)$ are shown as functions of p for selected values of z . The two functions are equal to within the accuracy of the graph except where indicated by splitting of the lines.

The surface thickness, which is the distance in which the particle density rises from 10% to 90% of its asymptotic value in the interior, is 2.01 fermis. This may be compared with a value of 2.5 ± 0.2 fermis obtained from high-energy electron-scattering data.⁽¹⁰⁾

Figure 2 also gives the results for $V_0(z)$ from some of the earlier iterations. During the later iterations the solution has converged except for a slow drift backwards along the Z -axis, which is probably due to numerical errors in the spatial boundary conditions.

A detailed discussion of the more important numerical methods which were used is given in Appendix A.

CHAPTER IV

THE PUFF-MARTIN APPROXIMATION IN THE HOMOGENEOUS CASE

IV.1. General Derivation

Chapters IV and V present solutions for homogeneous and inhomogeneous nuclear matter in an approximation which takes into account certain two-particle correlation effects and is capable of describing the saturative effects of a repulsive core in the interparticle potential. This approximation was developed by Martin and Schwinger⁽¹⁾ and applied to homogeneous nuclear matter by Puff,⁽²⁾ who also gives a discussion of its accuracy. The derivation given here differs from Puff's derivation in that the use of a Fourier series in energy is avoided and the Fourier transformation of spatial variables is postponed until a later step. However, the resulting equations for the homogeneous case agree with those obtained by Puff.

For the sake of clarity, the following derivations parallel the presentation of the Hartree approximation as closely as possible. Use will be made of certain results from the preceding chapters which are generally valid and not limited to the Hartree case.

To simplify the notation, let the numerical variable k represent the set ζ_k, r_k, t_k , and let (dk) represent summation and infinite integration over these variables. In this notation (2.1) becomes

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G_1(1; 1') + i \int (d2)(d\bar{1})(d\bar{2}) \langle 12 | v | \bar{1} \bar{2} \rangle G_2(\bar{1} \bar{2}; 1'2^+) = \delta(1; 1') \quad , \quad (4.1)$$

where

$$\langle 12 | v | \bar{1} \bar{2} \rangle = \langle r_1 r_2 | v | \bar{r}_1 \bar{r}_2 \rangle \delta(t_1 - \bar{t}_1) \delta(t_2 - \bar{t}_2) \delta(t_1 - t_2) \quad . \quad (4.2)$$

The analogous equation for G_2 is

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G_2(12; 1'2') + i \int (d3)(d\bar{1})(d\bar{3}) \langle 13 | v | \bar{1} \bar{3} \rangle G_3(\bar{1} \bar{2} \bar{3}; 1'2'3^+) = \delta(1; 1') G_1(2; 2') - \delta(1; 2') G_1(2; 1') \quad . \quad (4.3)$$

Equations (4.1) and (4.3) may be combined into an equation for the difference between G_2 and the Hartree-Fock approximation $G_1 G_1 - G_1 G_1$,

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] [G_2(1\ 2; 1' 2') - G_1(1; 1') G_1(2; 2') + G_1(1; 2') G_1(2; 1')] =$$

$$-i \int (d3)(d\bar{1})(d\bar{3}) \langle 1\ 3 | v | \bar{1} \bar{3} \rangle$$

$$\times [G_3(\bar{1}\ 2\ \bar{3}; 1' 2' 3^+) - G_2(\bar{1}\ \bar{3}; 1' 3^+) G_1(2; 2') + G_2(\bar{1}\ \bar{3}; 2' 3^+) G_1(2; 1')] \quad (4.4)$$

By applying the differential operator $[i (\partial/\partial t_2) + (\nabla_2^2/2m) + \mu]$ to this equation, and using (4.1) and the equation for G_3 ,

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G_3(1\ 2\ 3; 1' 2' 3') + i \int (d4)(d\bar{1})(d\bar{4}) \langle 1\ 4 | v | \bar{1} \bar{4} \rangle G_4(\bar{1}\ 2\ 3\ \bar{4}; 1' 2' 3' 4^+) =$$

$$\delta(1; 1') G_2(2\ 3; 2' 3') - \delta(1; 2') G_2(2\ 3; 1' 3') + \delta(1; 3') G_2(2\ 3; 1' 2') \quad (4.5)$$

we may obtain an equation for G_2 which is symmetric in the variables 1 and 2,

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] \left[i \frac{\partial}{\partial t_2} + \frac{\nabla_2^2}{2m} + \mu \right] [G_2(1\ 2; 1' 2') - G_1(1; 1') G_1(2; 2') + G_1(1; 2') G_1(2; 1')] =$$

$$-i \int (d\bar{1})(d\bar{2}) \langle 1\ 2 | v | \bar{1} \bar{2} \rangle G_2(\bar{1}\ \bar{2}; 1' 2') =$$

$$- \int (d\bar{1})(d\bar{2})(d3)(d\bar{3})(d4)(d\bar{4}) \langle 1\ 3 | v | \bar{1} \bar{3} \rangle \langle 2\ 4 | v | \bar{2} \bar{4} \rangle$$

$$\times [G_4(\bar{1}\ \bar{2}\ \bar{3}\ \bar{4}; 1' 2' 3' 4^+) - G_2(\bar{1}\ \bar{3}; 1' 3^+) G_2(\bar{2}\ \bar{4}; 2' 4^+) + G_2(\bar{1}\ \bar{3}; 2' 3^+) G_2(\bar{2}\ \bar{4}; 1' 4^+)] \quad (4.6)$$

The Puff-Martin approximation is obtained by neglecting the right-hand side of this equation. This is equivalent to approximating G_4 by a combination of G_2 's which retains the two-particle correlations between the pairs of particles (1,3) and (2,4), which, in turn, are coupled by the interactions.

The approximate equation may be rewritten in integral form by using the free particle function G_1^0 which satisfies (4.1) with $v = 0$:

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G_1^0(1; 1') = \delta(1; 1') \quad (4.7)$$

In converting the approximation to an integral form, attention must be given to the periodic boundary conditions. Let us restrict τ to real values, limit the free variables t_1 , t_2 , t_1' , and t_2' to the interval 0 to τ , and

restrict the time integrations to 0 to τ (indicated by square brackets). Under these restrictions the approximation to (4.6) is equivalent to

$$\begin{aligned} G_2(1\ 2; 1' 2') &= G_1(1; 1') G_1(2; 2') - G_1(1; 2') G_1(2; 1') \\ &+ i \int [d1''] [d2''] G_1^0(1; 1'') G_1^0(2; 2'') \int [d\bar{1}] [d\bar{2}] \langle 1'' 2'' | v | \bar{1} \bar{2} \rangle \\ &\times G_2(\bar{1} \bar{2}; 1' 2') \quad , \end{aligned} \quad (4.8)$$

since operating on this equation with the appropriate differential operators gives (4.6), and the equation satisfies the boundary conditions on G_2 providing the G_1^0 's satisfy similar conditions.

The form of (4.8) reveals an asymmetry between unprimed and primed coordinates (as may be seen by expanding the equation in powers of the potential) which is a serious defect in the approximation, since it implies that the approximate G_1 and G_2 cannot simultaneously satisfy the G_1 equation (4.1) and its adjoint. This violates a set of conditions which have been shown by Baym and Kadanoff⁽¹¹⁾ to be sufficient to insure the conservations of particle number, momentum, energy, and angular momentum in a system which is subjected to an external disturbance. There is also reason to believe that this asymmetry is responsible for the violation of $\mu = dE_0/dN$ and the related ambiguities in the pressure, which will be discussed in Section IV.3.

The functions G_1 and G_2 are now determined by the simultaneous equations (4.1) and (4.8). In order to separate these equations, we introduce a subsidiary two-particle function Ω satisfying

$$\begin{aligned} \Omega(1\ 2; 1' 2') &= \delta(1; 1') \delta(2; 2') + i \int [d1''] [d2''] G_1^0(1; 1'') G_1^0(2; 2'') \\ &\times \int [d\bar{1}] [d\bar{2}] \langle 1'' 2'' | v | \bar{1} \bar{2} \rangle \Omega(\bar{1} \bar{2}; 1' 2') \quad , \end{aligned} \quad (4.9)$$

along with boundary conditions similar to those on G_2 . In terms of Ω , (4.8) has the solution

$$\begin{aligned} G_2(1\ 2; 1' 2') &= \int [d1''] [d2''] \Omega(1\ 2; 1'' 2'') \\ &[G_1(1''; 1') G_1(2''; 2') - G_1(1''; 2') G_1(2''; 1')] \quad , \end{aligned} \quad (4.10)$$

which gives G_2 explicitly in terms of G_1 . Substitution of this into (4.1) gives

$$\begin{aligned} \left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G_1(1; 1') + i \int [d2] [d\bar{1}] [d\bar{2}] [d1''] [d2''] \langle 1\ 2 | v | \bar{1} \bar{2} \rangle \\ \times [\Omega(\bar{1} \bar{2}; 1'' 2'') - \Omega(\bar{1} \bar{2}; 2'' 1'')] G_1(2''; 2') G_1(1''; 1') = \delta(1; 1') \quad . \end{aligned} \quad (4.11)$$

To solve (4.11), since v is local in time, the function $\Omega(12; 1'2')$ is needed only for $t_1 = t_2$. For this case, the substitution

$$\Omega(r_1 t_1 r_2 t_1; r_1' t_1' r_2' t_1') = \delta(t_1' - t_2') \Omega(r_1 r_2 t_1; r_1' r_2' t_1') \quad (4.12)$$

reduces (4.9) to

$$\begin{aligned} \Omega(r_1 r_2 t; r_1' r_2' t') &= \delta(t - t') \delta(r_1 - r_1') \delta(r_2 - r_2') \\ &+ i \int (dr_1'') (dr_2'') \int_0^\tau dt'' G_1^0(r_1 t; r_1'' t'') G_1^0(r_2 t; r_2'' t'') \\ &\times \int (d\bar{r}_1) (d\bar{r}_2) \langle r_1'' r_2'' | v | \bar{r}_1 \bar{r}_2 \rangle \Omega(\bar{r}_1 \bar{r}_2 t''; r_1' r_2' t') . \end{aligned} \quad (4.13)$$

We now wish to reconvert (4.13) into a differential equation by operating on it with $\left[i \frac{\partial}{\partial t} + \frac{\nabla_1^2 + \nabla_2^2}{2m} + 2\mu \right]$. We first note that the reduced Ω satisfies an even boundary condition, $\Omega(0 t') = +\Omega(\tau t')$, since both G_1^0 's in (4.13) change sign as t goes from 0 to τ . Secondly we may use (4.7) to obtain

$$\begin{aligned} \left[i \frac{\partial}{\partial t} + \frac{\nabla_1^2 + \nabla_2^2}{2m} + 2\mu \right] G_1^0(r_1 t; r_1' t') G_1^0(r_2 t; r_2' t') &= \\ \delta(t - t') [\delta(r_1 - r_1') G_1^0(r_2 t; r_2' t') + \delta(r_2 - r_2') G_1^0(r_1 t; r_1' t')] &, \end{aligned} \quad (4.14)$$

where

$$G_1^0(r t; r' t) = \frac{1}{2} [G_1^0(r t; r' t^+) + G_1^0(r t; r' t^-)] . \quad (4.15)$$

Since the Hartree-Fock derivation in Chapter II is exact for free particles, G_1^0 may be obtained by substituting the free-particle solution $A_0(p, \omega) = 2\pi\delta(\omega - (p^2/2m))$ into (2.17). This gives

$$G_1^0(r t; r' t) = \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot (r - r')} G_{00}(p) , \quad (4.16)$$

where

$$G_{00}(p) = \frac{1}{2i} \left[\coth \frac{i \left(\frac{p^2}{2m} - \mu \right) \tau}{2} \right]^{-1} . \quad (4.17)$$

Using these results, and replacing p by $\frac{1}{i}\nabla$ to indicate Fourier transformation, we obtain the desired differential equation. Equation (4.13) is equivalent to

$$\left[i \frac{\partial}{\partial t} + \frac{\nabla_1^2 + \nabla_2^2}{2m} + 2\mu \right] \left[\Omega(r_1 r_2 t; r'_1 r'_2 t') - \delta(t - t') \delta(r_1 - r'_1) \delta(r_2 - r'_2) \right] =$$

$$i \left[G_{00} \left(\frac{\nabla_1}{i} \right) + G_{00} \left(\frac{\nabla_2}{i} \right) \right] \int (d\bar{r}_1)(d\bar{r}_2) \langle r_1 r_2 | v | \bar{r}_1 \bar{r}_2 \rangle \times \Omega(\bar{r}_1 \bar{r}_2 t; r'_1 r'_2 t') , \quad (4.18)$$

along with the even boundary condition on Ω . If we introduce sum and difference coordinates,

$$R = \frac{r_1 + r_2}{2} ; \quad r = r_1 - r_2 ; \quad \nabla_1 = \frac{\nabla_R}{2} + \nabla_r ;$$

$$\nabla_2 = \frac{\nabla_R}{2} - \nabla_r , \quad (4.19)$$

and use

$$\langle r_1 r_2 | v | r'_1 r'_2 \rangle = v(r, r') \delta(R - R') , \quad (4.20)$$

then (4.18) becomes

$$\left[i \frac{\partial}{\partial t} + \frac{\nabla_R^2}{4m} + \frac{\nabla_r^2}{m} + 2\mu \right] \left[\Omega[R, r, t; R', r', t'] - \delta(t - t') \delta(R - R') \delta(r - r') \right] =$$

$$i \left[G_{00} \left(\frac{\nabla_R}{2i} + \frac{\nabla_r}{i} \right) + G_{00} \left(\frac{\nabla_R}{2i} - \frac{\nabla_r}{i} \right) \right]$$

$$\times \int (d\bar{r}) v(r, \bar{r}) \Omega[R, \bar{r}, t; R', r', t'] , \quad (4.21)$$

where the square brackets indicate sum and difference coordinates as in (3.2).

Now Ω is the solution of a linear equation whose kernel is spatially homogeneous, and therefore Ω itself is spatially homogeneous, even when G_1 is not. Thus we may introduce the Fourier transform

$$\Omega[R, r, t; R', r', t'] = \int \frac{(dP)}{(2\pi)^3} e^{iP \cdot (R - R')} \Omega(P, r, t; r', t') , \quad (4.22)$$

which reduces (4.21) to

$$\left[i \frac{\partial}{\partial t} - \frac{P^2}{4m} + \frac{\nabla_r^2}{m} + 2\mu \right] \left[\Omega(P, r, t; r', t') - \delta(r - r') \delta(t - t') \right] =$$

$$\int (d\bar{r}) \bar{v}(P, r, \bar{r}) \Omega(P, \bar{r}, t; r', t') , \quad (4.23)$$

where

$$\bar{v}(\mathbf{P} \mathbf{r} \bar{\mathbf{r}}) = i \left[G_{00} \left(\frac{\mathbf{P}}{2} + \frac{\nabla_{\mathbf{r}}}{i} \right) + G_{00} \left(\frac{\mathbf{P}}{2} - \frac{\nabla_{\mathbf{r}}}{i} \right) \right] v(\mathbf{r} \bar{\mathbf{r}}) \quad (4.24)$$

We note that in the low-temperature limit as $i\tau \rightarrow \infty$, providing $\mu < 0$ (which is the case for nuclear matter), the hyperbolic cotangents in G_{00} will go to one, and $\bar{v}(\mathbf{P} \mathbf{r} \mathbf{r}')$ will reduce to $v(\mathbf{r} \mathbf{r}')$.

Equation (4.23) has the solution

$$\Omega(\mathbf{P} \mathbf{r} \mathbf{t}; \mathbf{r}' \mathbf{t}') = \delta(\mathbf{r} - \mathbf{r}') \delta(\mathbf{t} - \mathbf{t}') + \int (d\mathbf{r}'') \mathcal{G}(\mathbf{P} \mathbf{r} \mathbf{t}; \mathbf{r}'' \mathbf{t}') \bar{v}(\mathbf{P} \mathbf{r}'' \mathbf{r}') \quad , \quad (4.25)$$

where \mathcal{G} is the Green's function satisfying

$$\left[i \frac{\partial}{\partial \mathbf{t}} - \frac{\mathbf{P}^2}{4m} + \frac{\nabla_{\mathbf{r}}^2}{m} + 2\mu \right] \mathcal{G}(\mathbf{P} \mathbf{r} \mathbf{t}; \mathbf{r}' \mathbf{t}') - \int (d\bar{\mathbf{r}}) \bar{v}(\mathbf{P} \mathbf{r} \bar{\mathbf{r}}) \mathcal{G}(\mathbf{P} \bar{\mathbf{r}} \mathbf{t}; \mathbf{r}' \mathbf{t}') = \delta(\mathbf{r} - \mathbf{r}') \delta(\mathbf{t} - \mathbf{t}') \quad , \quad (4.26)$$

along with the same even boundary conditions as Ω . The function \mathcal{G} may be expressed in spectral form by a process similar to (2.12) to (2.19), but using the even boundary condition instead of (2.13). The result is

$$\mathcal{G}(\mathbf{P} \mathbf{r} \mathbf{t}; \mathbf{r}' \mathbf{t}') = \frac{1}{i} \int \frac{d\omega}{2\pi} e^{-i\left(\omega - 2\mu + \frac{\mathbf{P}^2}{4m}\right)(\mathbf{t} - \mathbf{t}')} \times \begin{cases} \frac{\mathcal{A}(\mathbf{P} \mathbf{r} \mathbf{r}' \omega)}{1 - e^{-i(\omega - 2\mu + \mathbf{P}^2/4m)\tau}} ; & \mathbf{t} > \mathbf{t}' \\ - \frac{\mathcal{A}(\mathbf{P} \mathbf{r} \mathbf{r}' \omega)}{1 - e^{+i(\omega - 2\mu + \mathbf{P}^2/4m)\tau}} ; & \mathbf{t} < \mathbf{t}' \end{cases} \quad , \quad (4.27)$$

where \mathcal{A} satisfies

$$\left(\omega + \frac{\nabla_{\mathbf{r}}^2}{m} \right) \mathcal{A}(\mathbf{P} \mathbf{r} \mathbf{r}' \omega) - \int (d\bar{\mathbf{r}}) \bar{v}(\mathbf{P} \mathbf{r} \bar{\mathbf{r}}) \mathcal{A}(\mathbf{P} \bar{\mathbf{r}} \mathbf{r}' \omega) = 0 \quad (4.28)$$

and the normalization condition

$$\int \frac{d\omega}{2\pi} \mathcal{A}(\mathbf{P} \mathbf{r} \mathbf{r}' \omega) = \delta(\mathbf{r} - \mathbf{r}') \quad . \quad (4.29)$$

From (4.28) we may infer that \mathcal{Q} is composed of wave functions of the reduced-mass system of two particles with an interparticle potential $\bar{v}(\mathbf{P} \mathbf{r} \mathbf{r}')$. It will be useful to define a scattering matrix in terms of \mathcal{Q} :

$$\langle \mathbf{r} | \bar{t}(\mathbf{P} \omega) | \mathbf{r}' \rangle = v(\mathbf{r} \mathbf{r}') + \int (d\mathbf{r}'') (d\mathbf{r}''') v(\mathbf{r} \mathbf{r}'') \int \frac{d\omega'}{2\pi} \frac{\mathcal{Q}(\mathbf{P} \mathbf{r}'' \mathbf{r}''' \omega')}{\omega - \omega'} \bar{v}(\mathbf{P} \mathbf{r}''' \mathbf{r}') . \quad (4.30)$$

As $i\tau \rightarrow \infty$ and $\bar{v} \rightarrow v$, the quantity \bar{t} becomes the conventional two-body scattering matrix for the potential v .

Having obtained the function Ω , we now substitute our result into (4.11). Using (4.2), (4.20), (4.12), (4.22), and (4.25), we obtain

$$\begin{aligned} & \left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G_1(\mathbf{r}_1 t; \mathbf{r}_1' t') \\ & + i \int (d\mathbf{r}_1'') (d\mathbf{r}_2'') \delta(\mathbf{R} - \mathbf{R}'') v_{\text{sym}}(\mathbf{r} \mathbf{r}'') G_1(\mathbf{r}_2'' t; \mathbf{r}_2 t^+) G_1(\mathbf{r}_1'' t; \mathbf{r}_1' t') \\ & + i \int_0^\tau dt'' \int (d\mathbf{r}_1'') (d\mathbf{r}_2'') \frac{(d\mathbf{P})}{(2\pi)^3} e^{i\mathbf{P} \cdot (\mathbf{R} - \mathbf{R}'')} \int (d\bar{\mathbf{r}}) (d\bar{\mathbf{r}}') v(\mathbf{r} \bar{\mathbf{r}}) \\ & \times \mathcal{Q}(\mathbf{P} \bar{\mathbf{r}} t; \bar{\mathbf{r}}' t'') \bar{v}_{\text{sym}}(\mathbf{P} \bar{\mathbf{r}} \mathbf{r}'') G_1(\mathbf{r}_2'' t''; \mathbf{r}_2 t^+) G_1(\mathbf{r}_1'' t''; \mathbf{r}_1' t') = \\ & \delta(\mathbf{r}_1 - \mathbf{r}_1') \delta(t - t') , \end{aligned} \quad (4.31)$$

where

$$v_{\text{sym}}(\mathbf{r} \mathbf{r}') = v(\mathbf{r}, \mathbf{r}') - v(\mathbf{r}, -\mathbf{r}') , \quad (4.32)$$

and similarly for \bar{v} . In (4.31) the space variables without numerical subscripts are sum and difference coordinates defined as in (4.19). Except for the last term on the left-hand side, (4.31) is equivalent to the Hartree-Fock equations (2.3) and (2.4). The correlation effects are described by the additional term, which is nonlocal in time.

We now wish to derive an equation for the spectral function A . Equations (2.11) to (2.17) and (2.19) are still valid, but the simple procedure which led to (2.18) is no longer applicable because of the non-locality of the additional term in (4.31). Instead, to obtain an equation for A we may proceed as follows: Let

$$V_0(\mathbf{r}_1 \mathbf{r}_1') = -i \int (d\mathbf{r}_2) (d\mathbf{r}_2') \delta(\mathbf{R} - \mathbf{R}') v_{\text{sym}}(\mathbf{r} \mathbf{r}') G_1(\mathbf{r}_2' t; \mathbf{r}_2 t^+) , \quad (4.33)$$

and

$$U(r_1 t; r_1' t') = -i \int (dr_2)(dr_2') \frac{(dP)}{(2\pi)^3} e^{iP \cdot (R - R')} \\ \times \int (dr''')(dr''') v(r r''') \mathcal{G}(P r'' t; r''' t') \bar{v}_{\text{sym}}(P r''' r') G_1(r_2' t'; r_2 t) . \quad (4.34)$$

Using these functions and suppressing the spatial coordinates into a matrix notation, we may write (4.31) as

$$\left[i \frac{\partial}{\partial t} + \frac{\nabla_1^2}{2m} + \mu - V_0 \right] G_1(t t') - \int_0^\tau dt'' U(t t'') G_1(t'' t') = \delta(t - t') \quad . \quad (4.35)$$

We introduce the functions $G_>$ and $G_<$ defined by (2.11) and satisfying (2.12) and (2.13). Similarly, we define $U_>$ and $U_<$ by

$$U(t t') = \begin{cases} U_>(t t') & ; \quad t > t' \\ U_<(t t') & ; \quad t < t' \end{cases} , \quad (4.36)$$

and in the remaining regions of t and t' by analytic continuation. Now, the independent time variables have been restricted to the interval 0 to τ . If we impose the additional restriction $t' < t$, then the substitution of (2.12) and (4.36) reduces (4.35) to

$$\left[i \frac{\partial}{\partial t} + \frac{\nabla_1^2}{2m} + \mu - V_0 \right] G_>(t t') - \int_0^{t'} dt'' U_>(t t'') G_<(t'' t') \\ - \int_{t'}^t dt'' U_>(t t'') G_>(t'' t') - \int_t^\tau dt'' U_<(t t'') G_>(t'' t') = 0 \quad . \quad (4.37)$$

But, unlike (4.35), equation (4.37) is an analytic equation in analytic functions. Therefore it must hold, not only in the region $0 < t' < t < \tau$, but throughout the entire range of t and t' .

Because of (2.13) and the analogous even condition on \mathcal{G} , (4.34) implies that

$$U_<(t, t') = -U_>(t + \tau, t') \quad . \quad (4.38)$$

The substitution of this result and (2.13) into (4.37) to eliminate $U_{<}$ and $G_{<}$ gives

$$\left[i \frac{\partial}{\partial t} + \frac{\nabla_1^2}{2m} + \mu - V_0 \right] G_{>}(t t') - \int_{t'}^t dt'' U_{>}(t t'') G_{>}(t'' t') \\ + \int_t^{\tau + t'} dt'' U_{>}(t + \tau, t'') G_{>}(t'' t') = 0 \quad . \quad (4.39)$$

If we introduce the Fourier transform of $G_{>}$ given by (2.14) and the analogous transform of $U_{>}$,⁽⁵⁾

$$U_{>}(t t') = \int \frac{d\omega}{2\pi i} e^{-i(\omega - \mu)(t - t')} u_{>}(\omega) \quad (4.40)$$

(since $U_{>}$ depends only on $t - t'$), we may transform (4.39) into

$$\left(\omega + \frac{\nabla_1^2}{2m} - V_0 \right) g_{>}(\omega) - \int \frac{d\omega'}{2\pi} \frac{d\omega''}{2\pi} \left[\frac{1}{i} \int dt \int_0^t dt'' e^{i(\omega - \omega')t + i(\omega' - \omega'')t''} \right. \\ \left. - \frac{1}{i} e^{-i(\omega' - \mu)\tau} \int dt \int_t^\tau dt'' e^{i(\omega - \omega')t + i(\omega' - \omega'')t''} \right] u_{>}(\omega') g_{>}(\omega'') = 0 \quad . \quad (4.41)$$

The quantity in square brackets is equal to

$$2\pi \frac{1}{\omega'' - \omega'} \left[(1 + e^{-i(\omega' - \mu)\tau}) \delta(\omega - \omega'') - (1 + e^{-i(\omega'' - \mu)\tau}) \delta(\omega - \omega') \right], \quad (4.42)$$

so that (4.41) is just

$$\left(\omega + \frac{\nabla_1^2}{2m} - V_0 \right) g_{>}(\omega) \\ - P \int \frac{d\omega'}{2\pi} \frac{1}{\omega - \omega'} [1 + e^{-i(\omega' - \mu)\tau}] [u_{>}(\omega') g_{>}(\omega) + u_{>}(\omega) g_{>}(\omega')] = 0 \quad . \quad (4.43)$$

Here P indicates that the principal part of the integral is to be used, as may be verified by replacing the denominator in (4.42) by $\omega'' - \omega' + i\epsilon$, substituting into (4.41), and using

$$\frac{1}{\omega \mp i\epsilon} = P \frac{1}{\omega} \mp \pi i \delta(\omega) \quad . \quad (4.44)$$

We now express $g_{>}$ in terms of A by using (2.16), and treat $u_{>}$ analogously by defining a function $B(\omega)$ such that

$$u_{>}(\omega) = \frac{B(\omega)}{1 + e^{-i(\omega - \mu)\tau}} . \quad (4.45)$$

Finally the substitution of (2.16) and (4.45) into (4.43) gives the desired equation for A :

$$\left[\omega + \frac{\nabla_1^2}{2m} - V_0 \right] A(\omega) - P \int \frac{d\omega'}{2\pi} \frac{1}{\omega - \omega'} [B(\omega') A(\omega) + B(\omega) A(\omega')] = 0 . \quad (4.46)$$

We may define a function which is analogous to the effective potential in the Hartree approximation by

$$V(\omega) = V_0 + \int \frac{d\omega'}{2\pi} \frac{B(\omega')}{\omega - \omega'} , \quad (4.47)$$

where ω may be complex. The increased complexity of the Puff-Martin approximation is expressed by the energy dependence of this function. In general, $V(\omega)$ will have a discontinuity across the real axis at ω if $B(\omega) \neq 0$. For regions of ω in which there is no discontinuity, i.e., in which $B(\omega) = 0$, equation (4.46) reduces to the simple form

$$\left[\omega + \frac{\nabla_1^2}{2m} - V(\omega) \right] A(\omega) = 0 , \quad (4.48)$$

or, explicitly,⁽⁵⁾

$$\left[\omega + \frac{\nabla_1^2}{2m} \right] A(r_1 r_1' | \omega) - \int (dr_1'') V(r_1 r_1'' | \omega) A(r_1'' r_1' | \omega) = 0 , \quad (4.49)$$

which is analogous to the Hartree equation (2.18), and which permits a wave-function expansion similar to (2.20) and (2.21).

Although we will need to find $A(\omega)$ only in the region of ω in which V is continuous, we will need to deal with the general situation in order to normalize A . In this case, it is useful to define an energy Green's function (for complex ω):

$$G(\omega) = \int \frac{d\omega'}{2\pi} \frac{A(\omega')}{\omega - \omega'} . \quad (4.50)$$

Replacing ω by ω'' and performing the operation $\int \frac{d\omega''}{2\pi} \frac{1}{\omega - \omega''}$ (for complex ω) on (4.46) gives

$$\begin{aligned}
 & - \int \frac{d\omega''}{2\pi} A(\omega'') + \left(\omega + \frac{\nabla_1^2}{2m} - V_0 \right) G(\omega) \\
 & - \int \frac{d\omega''}{2\pi} \int \frac{d\omega'}{2\pi} \frac{1}{\omega - \omega''} \frac{1}{\omega'' - \omega'} [B(\omega') A(\omega'') + B(\omega'') A(\omega')] = 0 \quad (4.51)
 \end{aligned}$$

The first term may be evaluated by using the normalization condition (2.19). In the double integral the symmetry of $(BA + AB)$ in ω' and ω'' allows the replacement

$$\frac{1}{\omega - \omega''} \frac{1}{\omega'' - \omega'} \rightarrow \frac{1}{2} \left[\frac{1}{\omega - \omega''} \frac{1}{\omega'' - \omega'} + \frac{1}{\omega - \omega'} \frac{1}{\omega' - \omega''} \right] = \frac{1}{2} \frac{1}{\omega - \omega'} \frac{1}{\omega - \omega''} \quad (4.52)$$

Thus, (4.51) reduces to

$$\left(\omega + \frac{\nabla^2}{2m} - V(\omega) \right) G(\omega) = 1 \quad (4.53)$$

Once this equation has been solved for $G(\omega)$, the function A may be extracted by using

$$A(\omega) = \int \frac{d\omega'}{2\pi i} \left[\frac{A(\omega')}{\omega - \omega' - i\epsilon} - \frac{A(\omega')}{\omega - \omega' + i\epsilon} \right] = \frac{1}{i} [G(\omega - i\epsilon) - G(\omega + i\epsilon)] \quad (4.54)$$

We still need to express $V(\omega)$ in terms of $A(\omega)$. By substituting (2.17) and (4.27) into (4.34), and using (4.36), the inverse of (4.40), and (4.45), we obtain

$$\begin{aligned}
 B(r_1 r_1' \omega) &= \int \frac{d\omega'}{2\pi} (dr_2)(dr_2') \frac{(dP)}{(2\pi)^3} e^{iP \cdot (R - R')} \int (dr'')(dr''') v(r r'') \\
 &\times a \left(P r'' r''', \omega + \omega' - \frac{P^2}{4m} \right) \bar{v}_{\text{sym}}(P r''' r') A(r_2' r_2 \omega') \\
 &\times \left[\frac{1 + e^{-i(\omega - \mu)\tau}}{(1 - e^{-i(\omega + \omega' - 2\mu)\tau})(1 + e^{i(\omega' - \mu)\tau})} \right] \quad (4.55)
 \end{aligned}$$

where the factor in square brackets reduces to

$$\frac{1}{1 - e^{-i(\omega + \omega' - 2\mu)\tau}} - \frac{1}{1 + e^{-i(\omega' - \mu)\tau}} \quad (4.56)$$

We must find the low-temperature limit of (4.55) as $i\tau \rightarrow \infty$ and $\bar{v} \rightarrow v$. This limit will be greatly simplified if we may assume that $2\mu < \omega_0$, where $\omega_0 = -2.225$ Mev, is the binding energy of the deuteron. We will find this assumption to be justified for nuclear matter at reasonable densities.

Now the function \mathcal{A} is zero when $\omega + \omega' - (P^2/4m) < \omega_0$, since ω_0 is the lowest eigenvalue of equation (4.28). Thus if $2\mu < \omega_0$, then $\mathcal{A} = 0$ for $\omega + \omega' \leq 2\mu$, and we need only consider the region $\omega + \omega' > 2\mu$ in taking the limit of (4.56) as $i\tau \rightarrow \infty$. In this region the limit is $\mathcal{N} - (\omega' - \mu)$, and substitution into (4.55) gives

$$B(r_1 r_1' \omega) = \int^\mu \frac{d\omega'}{2\pi} (dr_2)(dr_2') \frac{(dP)}{(2\pi)^3} e^{iP \cdot (R - R')} \int (dr'')(dr''') \\ \times v(r r'') \mathcal{A}(r'' r''', \omega + \omega' - \frac{P^2}{4m}) v_{\text{sym}}(r''' r') A(r_2' r_2 \omega') \quad (4.57)$$

Since \mathcal{A} is zero for $\omega + \omega' - (P^2/4m) < \omega_0$, then $B(\omega)$ is zero for $\omega < \omega_0 - \mu$, and in this region $V(\omega)$ will be continuous. But on the other hand, to determine $B(\omega)$ from (4.57) we need to know $A(\omega)$ only for $\omega < \mu$. If we again assume $2\mu < \omega_0$, then this region is entirely within the region in which $V(\omega)$ is continuous, and a self-consistent solution for $V(\omega)$ can be obtained without finding $A(\omega)$ in the discontinuous region of V .

Substituting (4.57), (4.33) and (2.17) into (4.47), and using (4.30), we finally obtain

$$V(r_1 r_1' \omega) = \int^\mu \frac{d\omega'}{2\pi} (dr_2)(dr_2') \frac{(dP)}{(2\pi)^3} e^{iP \cdot (R - R')} \\ \times \langle r | t_{\text{sym}} \left(\omega + \omega' - \frac{P^2}{4m} \right) | r' \rangle A(r_2' r_2 \omega') \quad (4.58)$$

where

$$\langle r | t_{\text{sym}}(\omega) | r' \rangle = \langle r | t(\omega) | r' \rangle - \langle r | t(\omega) | -r' \rangle \quad (4.59)$$

and $\langle r | t(\omega) | r' \rangle$ is the scattering matrix of the reduced-mass two-body system, defined by (4.28), (4.29), and (4.30) with $\bar{v}(P r r')$ replaced by $v(r r')$ to give the low-temperature limit.

In the preceding discussion we have ignored the presence of the internal variables of spin and isotopic spin. These variables may be made explicit by considering equation (4.11), which may be written as

$$\left[i \frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m} + \mu \right] G_1(1; 1') + i \int [d2][d1''] G_1(1; 1'') G_1(1''; 2') = \delta(1; 1') \quad , \quad (4.60)$$

where

$$\theta(1; 2; 1''; 2'') = \int [d\bar{1}][d\bar{2}] \langle 1; 2 | v | \bar{1}; \bar{2} \rangle \Omega(\bar{1}; \bar{2}; 1''; 2'') \quad . \quad (4.61)$$

Any two-particle function such as θ may be expanded in exchange operators in the internal variables, in the same manner as in equation (2.7):

$$\theta = \theta_0 1 + \theta_\sigma P^\sigma + \theta_\tau P^\tau + \theta_{\sigma\tau} P^\sigma P^\tau \quad . \quad (4.62)$$

The same reasoning as was used in Section II.1 leads to the conclusion that the internal variables may be accounted for by replacing the difference of θ 's in (4.60) by

$$\theta(1; 2; 1''; 2'') - \theta_{\text{ex}}(1; 2; 2''; 1'') \quad , \quad (4.63)$$

where

$$\begin{aligned} \theta &= 4\theta_0 + 2\theta_\sigma + 2\theta_\tau + \theta_{\sigma\tau} \quad ; \\ \theta_{\text{ex}} &= \theta_0 + 2\theta_\sigma + 2\theta_\tau + 4\theta_{\sigma\tau} \quad . \end{aligned} \quad (4.64)$$

In the Puff-Martin approximation it is convenient to replace the expansion of the two-particle functions in exchange operators by an expansion in singlet and triplet projection operators:

$$\theta = \theta_{ss} P_s^\sigma P_s^\tau + \theta_{ts} P_t^\sigma P_s^\tau + \theta_{st} P_s^\sigma P_t^\tau + \theta_{tt} P_t^\sigma P_t^\tau \quad , \quad (4.65)$$

where

$$\begin{aligned} P_s^\sigma &= \frac{1}{2} (1 - P^\sigma) \quad ; \quad P_t^\sigma = \frac{1}{2} (1 + P^\sigma) \quad ; \\ P_s^\tau &= \frac{1}{2} (1 - P^\tau) \quad ; \quad P_t^\tau = \frac{1}{2} (1 + P^\tau) \quad . \end{aligned} \quad (4.66)$$

If we substitute (4.66) into (4.65) and compare the result with (4.62), we obtain expressions for θ_0 , θ_σ , θ_τ , and $\theta_{\sigma\tau}$ in terms of θ_{ss} , θ_{ts} , θ_{st} , and θ_{tt} . Substitution of these into (4.64) gives

$$\begin{aligned}\theta &= \frac{1}{4} \theta_{ss} + \frac{3}{4} \theta_{ts} + \frac{3}{4} \theta_{st} + \frac{9}{4} \theta_{tt} ; \\ \theta_{ex} &= \frac{1}{4} \theta_{ss} - \frac{3}{4} \theta_{ts} - \frac{3}{4} \theta_{st} + \frac{9}{4} \theta_{tt} .\end{aligned}\quad (4.67)$$

The advantage of the singlet and triplet projection operators is their orthogonality. Because of this property, when an expression [such as (4.61)] which involves the folding of two-particle functions is expanded in the projection operators, the cross products of the operators vanish, and the expression holds separately for each of the four types of functions: ss, ts, st, and tt. Such a separation may be carried out throughout our entire derivation, and results in the replacement of (4.59) by a combination with the same form as (4.67):

$$\begin{aligned}\langle r | t_{\text{sym}} | r' \rangle &= \\ \frac{1}{4} \langle r | t_{ss} | r' \rangle &+ \frac{3}{4} \langle r | t_{ts} | r' \rangle + \frac{3}{4} \langle r | t_{st} | r' \rangle + \frac{9}{4} \langle r | t_{tt} | r' \rangle \\ - \frac{1}{4} \langle r | t_{ss} | -r' \rangle &+ \frac{3}{4} \langle r | t_{ts} | -r' \rangle + \frac{3}{4} \langle r | t_{st} | -r' \rangle - \frac{9}{4} \langle r | t_{tt} | -r' \rangle ,\end{aligned}\quad (4.68)$$

where the t 's on the right-hand side are two-body scattering matrices corresponding to the interparticle potentials v_{ss} , v_{ts} , v_{st} , and v_{tt} .

The equations (2.29) and (2.33), which express the particle and energy densities in terms of $A(\omega)$, are exact and still valid. (They must still be multiplied by a degeneracy factor of four.) Thus, in summary, we have the functions A and V determined by (4.48) [or (4.53) and (4.54)], (2.19), (4.58), and (4.68), where the particle and energy densities are given by (2.29) and (2.33).

IV. 2 - The Homogeneous Case

To obtain equations for the homogeneous case we introduce the spatial Fourier transforms of A and V as in (2.34) and (2.35):

$$A(r, r'; \omega) = \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot (r - r')} A(p, \omega) \quad (4.69)$$

and

$$V(r, r'; \omega) = \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot (r - r')} V(p, \omega) . \quad (4.70)$$

The transformation of (4.48) gives

$$\left[\omega - \frac{p^2}{2m} - V(p, \omega) \right] A(p, \omega) = 0 , \quad (4.71)$$

and (2.19) again becomes (2.37):

$$\int \frac{d\omega}{2\pi} A(p, \omega) = 1 \quad (4.72)$$

However, (2.40) and (2.41) are no longer correct, since the energy dependence of $V(p, \omega)$ prevents (2.40) from satisfying (4.72).

We might expect to resolve this difficulty by multiplying (2.40) by an unknown function of p and using (4.72) to determine this function. Unfortunately, this procedure is thwarted by the fact that (4.72) involves $A(p, \omega)$ for all ω , whereas (4.71) is valid only in the region of ω where $V(p, \omega)$ is continuous across the real axis. For this reason, we must resort to solving the general equations (4.53) and (4.54) for arbitrary ω and reducing these results for the case in which $V(\omega)$ is continuous.

Fortunately, this procedure is straightforward; the Fourier transform of (4.53) gives directly

$$G(p, \omega) = \frac{1}{\omega - \frac{p^2}{2m} - V(p, \omega)} \quad (4.73)$$

so that (4.54) becomes

$$A(\omega) = \frac{1}{i} \left[\frac{1}{\omega - i\epsilon - \frac{p^2}{2m} - V(p, \omega - i\epsilon)} - \frac{1}{\omega + i\epsilon - \frac{p^2}{2m} - V(p, \omega + i\epsilon)} \right] \quad (4.74)$$

In the special case in which V is continuous across the real axis, this expression is nonzero only in the neighborhood of $\omega = h(p)$, where $h(p)$ satisfies

$$h(p) = \frac{p^2}{2m} + V(p, h(p)) \quad (4.75)$$

[we assume $h(p)$ is single-valued]. Therefore, we may replace $V(p, \omega)$ in (4.74) by the first two terms of its Taylor expansion about $\omega = h(p)$:

$$V(p, \omega) \rightarrow V(p, h(p)) + (\omega - h(p)) \frac{\partial}{\partial \omega} V(p, h(p)) \quad (4.76)$$

obtaining the solution⁽⁵⁾

$$A(p, \omega) = \frac{1}{i} \left[1 - \frac{\partial}{\partial \omega} V(p, h(p)) \right]^{-1} \left[\frac{1}{\omega - h(p) - i\epsilon} - \frac{1}{\omega - h(p) + i\epsilon} \right] \\ = 2\pi \rho(p) \delta(\omega - h(p)) \quad (4.77)$$

where

$$\rho(p) = \left[1 - \frac{\partial}{\partial \omega} V(p, h(p)) \right]^{-1} \quad (4.78)$$

To express $V(p, \omega)$ in terms of $A(p, \omega)$ we must obtain the Fourier transform of (4.58). If we introduce the Fourier transform of a scattering matrix as

$$\langle r | t(\omega) | r' \rangle = \int \frac{(dp)(dp')}{(2\pi)^3} e^{ip \cdot r} \langle p | t(\omega) | p' \rangle e^{-ip' \cdot r'} \quad (4.79)$$

then, using (4.69), (4.70), and (4.79), we may transform (4.58) into⁽⁵⁾

$$V(p_1, \omega) = \int^\mu \frac{d\omega'}{2\pi} \int (dp_2) \left\langle \frac{p_1 - p_2}{2} \right| t_{\text{sym}} \left(\omega + \omega' - \frac{(p_1 + p_2)^2}{4m} \right) \left| \frac{p_1 - p_2}{2} \right\rangle \times A(p_2, \omega') \quad (4.80)$$

To facilitate the developments of Section IV.4 we write this equation as

$$V(p_1, \omega) = \int^\mu \frac{d\omega'}{2\pi} \int (dp_2) K(p_1, p_2, \omega + \omega') A(p_2, \omega') \quad (4.81)$$

where

$$K(p_1, p_2, \omega) = \int \frac{d\Omega}{4\pi} \left\langle \frac{p_1 - p_2}{2} \right| t_{\text{sym}} \left(\omega - \frac{(p_1 + p_2)^2}{4m} \right) \left| \frac{p_1 - p_2}{2} \right\rangle \quad (4.82)$$

and $\int \frac{d\Omega}{4\pi}$ is a spherical averaging over the angle between \vec{p}_1 and \vec{p}_2 .

Substitution of (4.77) into (4.81) gives

$$V(p_1, \omega) = \int_\Gamma (dp_2) K(p_1, p_2, \omega + h(p_2)) \rho(p_2) \quad (4.83)$$

where Γ is the region of momentum space where $\mu - h(p) > 0$. As in the Hartree case, we assume this region to be a sphere⁽¹²⁾ and designate its radius as the Fermi momentum p_f , which must satisfy $\mu - h(p_f) = 0$ or

$$\mu = h(p_f) = \frac{p_f^2}{2m} + V(p_f, h(p_f)) \quad (4.84)$$

The simultaneous solution of (4.83), (4.78), and (4.84) is simplified by introducing a potential function of momentum alone:

$$V(p) = V(p, h(p)) \quad (4.85)$$

In terms of this function, (4.83) becomes

$$V(p_1) = \int_{|p_2| < p_f} (dp_2) K(p_1, p_2, \frac{p_1^2 + p_2^2}{2m} + V(p_1) + V(p_2)) \rho(p_2) \quad (4.86)$$

(4.78) becomes

$$\rho(p_1) = \left[1 - \int_{|p_2| < p_f} (dp_2) \frac{\partial}{\partial \omega} K(p_1, p_2, \frac{p_1^2 + p_2^2}{2m} + V(p_1) + V(p_2)) \rho(p_2) \right]^{-1} \quad (4.87)$$

and (4.84) becomes

$$\mu = \frac{p_f^2}{2m} + V(p_f) \quad (4.88)$$

In addition, by substituting (4.69), (4.75), and (4.77) into (2.29) and (2.33), we may obtain expressions for the particle and energy densities:

$$\rho = \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \rho(p) \quad (4.89)$$

and

$$\epsilon = \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \left[\frac{p^2}{2m} + \frac{1}{2} V(p) \right] \rho(p) \quad (4.90)$$

With the substitution of (4.82), these equations agree with those obtained for the homogeneous case by Puff.⁽²⁾

We will not attempt to obtain the general requirements for saturation, which are extremely complicated in this approximation. It is sufficient to note that equations (4.86) and (4.87) are sensitive to the detailed shape of the interparticle potential, so that the dilemma which appeared in the Hartree-Fock case no longer occurs.

For a given p_f , the simultaneous equations (4.86) and (4.87) determine the functions $V(p)$ and $\rho(p)$, which, in turn, determine the chemical potential, and the particle and energy densities through equations (4.88) to (4.90). We will postpone the determination of the zero-pressure point until the next section, and limit ourselves for the moment to determining μ , ρ , and ϵ as functions of p_f .

To keep the numerical solution of these equations reasonably tractable, it is necessary to choose an interparticle potential for which the scattering matrix may be found algebraically. We follow Puff⁽²⁾ in choosing a potential which is the sum of three separable terms, an S-state hard shell and two Yamaguchi potentials⁽¹³⁾ acting on singlet and triplet spin states:

$$v = v_c + v_{yc}P_s^\sigma + v_{yt}P_t^\sigma, \quad (4.91)$$

where

$$v_c(r, r') = \lim_{\lambda_c \rightarrow \infty} \frac{\pi \lambda_c}{2m} \frac{1}{rr'} \delta(r - r_c) \delta(r' - r_c) \quad (4.92)$$

and

$$v_{y(s \text{ or } t)}(r, r') = -\frac{\pi}{2} \frac{\lambda_s \text{ or } t}{m} \frac{1}{rr'} e^{-\alpha_s \text{ or } t r} e^{-\alpha_s \text{ or } t r'} \quad (4.93)$$

Since this potential is independent of isotopic spin, the set of four potentials in the full singlet-triplet expansion of v consists of pairs of equal functions. Comparison of (4.91) with the general expansion (4.65) shows that

$$\begin{aligned} v_{ss} = v_{st} = v_s & \quad \text{where} \quad v_s = v_c + v_{ys} \\ v_{ts} = v_{tt} = v_t & \quad v_t = v_c + v_{yt} \end{aligned} \quad (4.94)$$

A similar equality relates the four scattering matrices t_{ss} , t_{st} , t_{ts} , and t_{tt} to the matrices t_s and t_t derived from v_s and v_t . Furthermore, since $v(r, r') = v(r, -r')$ for both potentials, we have $\langle r|t|r' \rangle = \langle r|t|-r' \rangle$ for each of the four t 's. This reduces (4.68) to

$$\begin{aligned} \langle r|t_{\text{sym}}|r' \rangle &= \frac{3}{2} \left[\langle r|t_{st}|r' \rangle + \langle r|t_{ts}|r' \rangle \right] \\ &= \frac{3}{2} \left[\langle r|t_s|r' \rangle + \langle r|t_t|r' \rangle \right], \end{aligned} \quad (4.95)$$

so that the effects of spin and isotopic spin are accounted for by simply summing the scattering matrices for singlet and triplet spins and multiplying by $3/2$.

The matrices t_s and t_t are determined by equations (4.28) to (4.30) (in the low-temperature limit). The solution of these equations for the

potentials in (4.92) to (4.94) is conveniently expressed by separating the energy and space dependence of the t 's. In this form the solution is

$$t(\omega) = \frac{1}{2m\pi} \left[\theta_{yy}(\omega) \tau_{yy} + \theta_{yc}(\omega) \tau_{yc} + \theta_{cc}(\omega) \tau_{cc} \right] , \quad (4.96)$$

where

$$\langle r | \tau | r' \rangle = \frac{1}{rr'} \begin{cases} e^{-\alpha r} e^{-\alpha r'} & (yy) \\ e^{-\alpha r} \delta(r' - r_c) + e^{-\alpha r'} \delta(r - r_c) & (yc) \\ \delta(r - r_c) \delta(r' - r_c) & (cc) \end{cases} , \quad (4.97)$$

or

$$\langle p | \tau | p' \rangle = \frac{2}{\pi} \begin{cases} \frac{1}{\alpha^2 + p^2} \frac{1}{\alpha^2 + p'^2} & (yy) \\ \frac{1}{\alpha^2 + p^2} \frac{\sin p' r_c}{p'} + \frac{\sin p r_c}{p} \frac{1}{\alpha^2 + p'^2} & (yc) \\ \frac{\sin p r_c}{p} \frac{\sin p' r_c}{p'} & (cc) \end{cases} , \quad (4.98)$$

and

$$\theta(\omega) = \left[\frac{1}{\gamma} \left(1 - \frac{\pi^2 \lambda}{\alpha(\alpha + \gamma)^2} \right) \left(1 - e^{-2\gamma r_c} \right) + \frac{4\pi^2 \lambda}{(\alpha^2 - \gamma^2)^2} (e^{-\gamma r_c} - e^{-\alpha r_c})^2 \right]^{-1} \\ \times \begin{cases} -\frac{\pi^2 \lambda}{\gamma} (1 - e^{-2\gamma r_c}) & (yy) \\ \frac{2\pi^2 \lambda}{\alpha^2 - \gamma^2} (e^{-\gamma r_c} - e^{-\alpha r_c}) & (yc) \\ \left(1 - \frac{\pi^2 \lambda}{\alpha(\alpha + \gamma)^2} \right) & (cc) \end{cases} , \quad (4.99)$$

and

$$\gamma = \sqrt{-m\omega} . \quad (4.100)$$

These expressions must be evaluated separately for the singlet and triplet spin states (using α_s , λ_s for t_s , and α_t , λ_t for t_t) and the resulting matrices combined according to (4.95) to obtain t_{sym} .

Puff⁽²⁾ has computed values of the parameters of v by fitting them to various scattering data and the binding energy of the deuteron. To permit the comparison of results, we have used his parameters, which are equivalent (in our units) to

$$\begin{aligned}
 \alpha_s &= 2.004 \text{ f}^{-1} & \lambda_s &= 3.64037 \text{ f}^{-3} & r_c &= 0.45 \text{ f} \\
 \alpha_t &= 2.453 \text{ f}^{-1} & \lambda_t &= 8.6949 \text{ f}^{-3}
 \end{aligned}
 \quad (4.101)$$

The IBM 704 was programmed to solve the equations for homogeneous matter for an interparticle potential of the form just discussed. By using Gaussian quadrature formulas, equations (4.86) and (4.87) were approximated by nonlinear matrix equations. These equations were solved by the following method:

1) The kernel $K(p_1 p_2 \omega)$ and its first two derivatives with respect to ω are obtained by numerical integration of the scattering matrix t_{sym} and its derivatives, as in (4.82).

2) By means of this kernel a table of $V(p)$ and $\rho(p)$ is obtained by solving the matrix equations corresponding to (4.86) and (4.87) for a particular value of p_f . This is done by iteration of a multidimensional Newton-Raphson procedure.

3) From this table the chemical potential, particle density, and energy density are obtained by using (4.88) to (4.90).

4) The entire procedure is repeated for a range of values of p_f .

This program was run with the use of the potential parameters in (4.101). The results of the calculations are shown in Figures 5 to 8 and tabulated in Appendix B. Figures 5 and 6 show the values of ϵ , ρ , μ , $E/N = \epsilon/\rho$, and $dE/dN = d\epsilon/d\rho$ (computed from the values of ϵ and ρ) as functions of p_f . Figures 7 and 8 show $V(p)$ and $\rho(p)$ for selected values of p_f . The results for E/N appear to agree with those given by Falk and Wilets⁽¹⁴⁾ for a more limited range of p_f .

As shown in Figure 6, the numerical results violate the relation $\mu = dE/dN$ which should hold for exact results. This failure is presumably a consequence of the asymmetry of G_2 in its unprimed and primed coordinates.

IV.3 - Computation of the Pressure

The results of our calculation specify the properties of nuclear matter as functions of the Fermi momentum p_f , or, equivalently, of the density. We must now determine the point on these curves which corresponds to zero pressure. In Chapter I we derived two expressions for the pressure: (1.23),

$$P = \rho \frac{d\epsilon}{d\rho} - \epsilon, \quad (4.102)$$

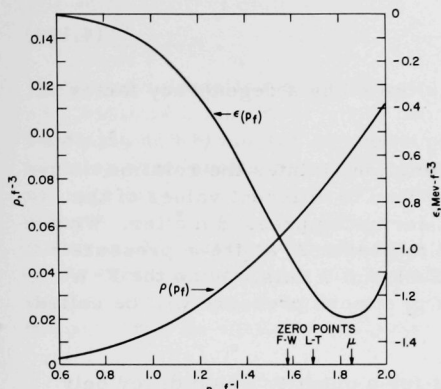


Fig. 5. Particle density ρ and energy density ϵ as functions of the Fermi momentum p_f , for homogeneous nuclear matter in the Puff-Martin approximation. Both ρ and ϵ must be multiplied by a degeneracy factor of 4.

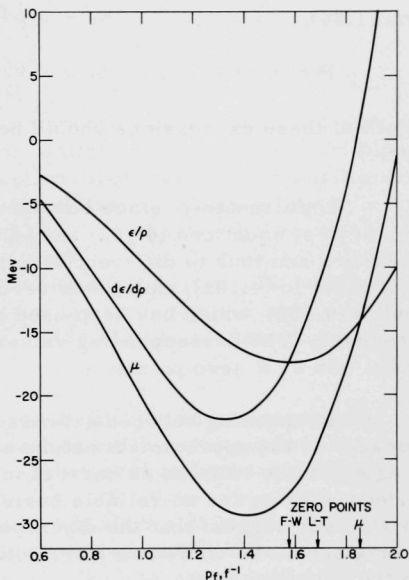


Fig. 6. Chemical potential μ , binding energy per particle ϵ/ρ , and the derivative of energy with respect to particle number at constant volume $d\epsilon/d\rho$ for homogeneous matter in the Puff-Martin approximation. All quantities are given as functions of the Fermi momentum p_f .

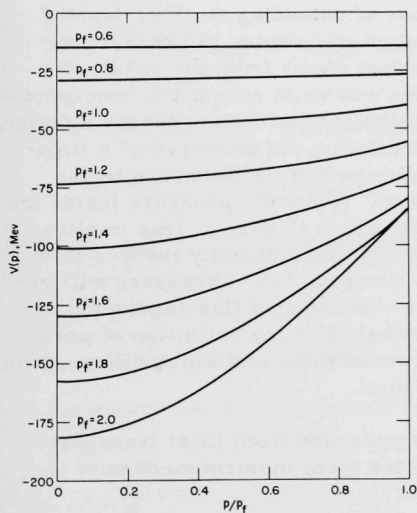


Fig. 7. Effective potential $V(p)$ of homogeneous nuclear matter in the Puff-Martin approximation, as a function of p/p_f for discrete values of p_f .

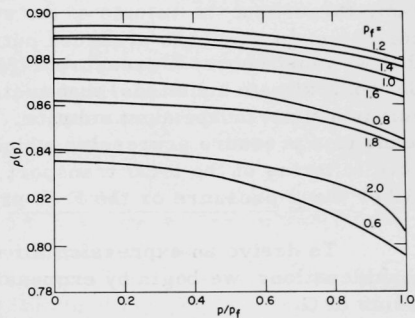


Fig. 8. Momentum distribution $\rho(p)$ of homogeneous nuclear matter in the Puff-Martin approximation, as a function of p/p_f for discrete values of p_f .

and (1.24),

$$P = \rho \mu - \epsilon \quad . \quad (4.103)$$

(Both of these expressions should be multiplied by a degeneracy factor of four.)

Unfortunately, since our approximation violates the relation $\mu = d\epsilon/d\rho$, equations (4.102) and (4.103) lead to different values of the pressure and thus to different densities for uncompressed matter. We will refer to (4.103), which was used in reference 2, as the μ pressure and to (4.102), which has been used by Falk and Wilets,⁽¹⁴⁾ as the F-W pressure. The corresponding values of p_f at zero pressure will be called the μ and F-W zero points.

In choosing between expressions for a quantity which differ only because of the approximate nature of a calculation, it is impossible to single out one relation as correct in any absolute and general sense. Indeed, we can see no reliable basis for preferring either (4.102) or (4.103) and suggest that the discrepancy between results at the two zero points should be viewed as a reflection of the inaccuracy which is inherent in the approximation.

However, for the specific purpose of extending the Puff-Martin approximation to an inhomogeneous system, the choice of pressure expressions is no longer arbitrary. This fact stems from the result of Chapter I that an inhomogeneous solution will exist only if the homogeneous solution which acts as a boundary condition on the inhomogeneous solution is evaluated at zero pressure. More precisely, the existence of a time-independent inhomogeneous solution requires that the pressure be the same throughout the volume of the system. (Thus the pressure inside the surface must equal the pressure outside, which is zero.) This implies that we must choose a pressure expression which directly insures (for the approximate equations) that spatial conservation of pressure will result in a time-independent solution. We will see that this requirement leads to a pressure expression which is based on the definition of pressure in terms of the local transport of momentum, and which differs from either the μ pressure or the F-W pressure.

To derive an expression for the pressure from local transport considerations, we begin by expressing the local momentum density in terms of G_1 :

$$\mathcal{G}(\mathbf{r}t) = \frac{1}{2i} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla - \nabla') \langle \psi^\dagger(\mathbf{r}'t) \psi(\mathbf{r}t) \rangle = -\frac{1}{2} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla - \nabla') G_1(\mathbf{r}t; \mathbf{r}'t^\dagger) \quad . \quad (4.104)$$

Then the time derivative of the momentum density is

$$\frac{\partial}{\partial t} \mathcal{G}(\mathbf{r}t) = \frac{i}{2} \lim_{\substack{\mathbf{r}' \rightarrow \mathbf{r} \\ t' \rightarrow t^+}} (\nabla - \nabla') \left[i \frac{\partial}{\partial t} + i \frac{\partial}{\partial t'} \right] G_1(\mathbf{r}t; \mathbf{r}'t') \quad . \quad (4.105)$$

To obtain an expression for the pressure, we must write (4.105) as the negative divergence of a stress tensor; the pressure will then be the average diagonal element of the stress tensor. By proceeding in this manner, we may insure that spatial conservation of the pressure will be a necessary condition for the time independence of G_1 (i.e., independence of the total time $t + t'$), since time independence will require that (4.105) vanish, which will, in turn, require that the stress tensor and, therefore, the pressure be spatially constant.

The essential point is that in deriving the stress tensor we must use equations which hold for the Puff-Martin approximation rather than for an exact calculation, since it is the approximate G_1 which must be time independent. In particular, to obtain the derivative $\partial G_1 / \partial t'$ in (4.105) we cannot use the adjoint of equation (4.1), since the asymmetry of our approximate G_2 in its unprimed and primed coordinates implies that the adjoint of (4.1) will not be satisfied. Instead, we may use the adjoint of (4.35):

$$\left[-i \frac{\partial}{\partial t'} + \frac{\nabla'^2}{2m} + \mu \right] G_1(\mathbf{r}t') - G_1(\mathbf{r}t') V_0 - \int_0^T dt'' G_1(\mathbf{r}t'') U(\mathbf{r}''t') = \delta(t - t') \quad , \quad (4.106)$$

since the symmetry of V_0 and U insures that (4.35) will imply its adjoint.

By substituting (4.35) and (4.106) into (4.105), we obtain

$$\begin{aligned} \frac{\partial}{\partial t} \mathcal{G}(\mathbf{r}t) = & -\frac{i}{2} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla - \nabla') \left\{ \frac{\nabla^2 - \nabla'^2}{2m} G_1(\mathbf{r}t^+) - V_0 G_1(\mathbf{r}t^+) + G_1(\mathbf{r}t^+) V_0 \right. \\ & \left. - \int_0^T dt'' \left[U(\mathbf{r}t'') G_1(\mathbf{r}''t^+) - G_1(\mathbf{r}t'') U(\mathbf{r}''t^+) \right] \right\} \quad , \quad (4.107) \end{aligned}$$

and the usual transformation from a time to an energy description gives

$$\frac{\partial}{\partial t} \mathcal{G}(\mathbf{r}t) = \frac{1}{2} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla - \nabla') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \left[\frac{\nabla^2 - \nabla'^2}{2m} A(\omega) - V(\omega) A(\omega) + A(\omega) V(\omega) \right] \quad . \quad (4.108)$$

We then write the time derivative of \mathcal{G} as a negative divergence of a stress tensor T , and divide T into a kinetic and a potential portion:

$$\frac{\partial}{\partial t} \mathcal{G}(\mathbf{r}t) = -\nabla \cdot T(\mathbf{r}) = -\nabla \cdot [T^{(0)}(\mathbf{r}) + T^{(1)}(\mathbf{r})] \quad (4.109)$$

where

$$\nabla \cdot T^{(0)}(\mathbf{r}) = -\frac{1}{2} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla - \nabla') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \frac{\nabla^2 - \nabla'^2}{2m} A(\mathbf{r} \mathbf{r}' \omega) \quad (4.110)$$

and

$$\begin{aligned} \nabla \cdot T^{(1)}(\mathbf{r}) = & \frac{1}{2} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla - \nabla') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \\ & \int (d\mathbf{r}'') \left[V(\mathbf{r} \mathbf{r}'' \omega) A(\mathbf{r}'' \mathbf{r}' \omega) - A(\mathbf{r} \mathbf{r}'' \omega) V(\mathbf{r}'' \mathbf{r}' \omega) \right]. \end{aligned} \quad (4.111)$$

Equation (4.110) determines the kinetic portion of the stress tensor to be

$$T^{(0)}(\mathbf{r}) = -\frac{1}{2} \frac{1}{2m} \lim_{\mathbf{r}' \rightarrow \mathbf{r}} (\nabla - \nabla') (\nabla - \nabla') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(\mathbf{r} \mathbf{r}' \omega) \quad (4.112)$$

However, the potential contribution to $\partial \mathcal{G} / \partial t$ cannot be generally expressed as a divergence. Nevertheless, for a short-range potential, it is possible to express this contribution as a divergence in a region of local uniformity. This may be done by integrating the potential contribution over a macroscopic region. We first use (4.58) to write (4.111) in terms of the scattering matrix and spectral function as

$$\begin{aligned} \nabla \cdot T^{(1)}(\mathbf{r}_1) = & \frac{1}{2} \lim_{\mathbf{r}_1' \rightarrow \mathbf{r}_1} (\nabla_1 - \nabla_1') \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \int_{-\infty}^{\mu} \frac{d\omega'}{2\pi} \int (d\mathbf{r}_1'') (d\mathbf{r}_2) (d\mathbf{r}_2') \\ & \left[\langle \mathbf{r}_1 \mathbf{r}_2 | T(\omega + \omega') | \mathbf{r}_1' \mathbf{r}_2' \rangle A(\mathbf{r}_2' \mathbf{r}_2 \omega') A(\mathbf{r}_1' \mathbf{r}_1' \omega) - A(\mathbf{r}_1 \mathbf{r}_1' \omega) \langle \mathbf{r}_1'' \mathbf{r}_2 | T(\omega + \omega') | \mathbf{r}_1' \mathbf{r}_2' \rangle A(\mathbf{r}_2' \mathbf{r}_2 \omega') \right] \end{aligned} \quad (4.113)$$

where

$$\langle \mathbf{r}_1 \mathbf{r}_2 | T(\omega) | \mathbf{r}_1' \mathbf{r}_2' \rangle = \int \frac{(d\mathbf{P})}{(2\pi)^3} e^{i\mathbf{P} \cdot (\mathbf{R} - \mathbf{R}')} \langle \mathbf{r} | t_{\text{sym}}(\omega - \mathbf{P}^2/4m) | \mathbf{r}' \rangle \quad (4.114)$$

Now, since T is independent of G_1 , it is a spatially homogeneous function, even for a system which is inhomogeneous. Using this fact and the symmetry of T and A in unprimed and primed coordinates, we obtain

$$\begin{aligned} \nabla \cdot T^{(1)}(\mathbf{r}_1) = & \int (d\mathbf{r}_1'') (d\mathbf{r}_2) (d\mathbf{r}_2') \langle \mathbf{r}_1 \mathbf{r}_2 | T | \mathbf{r}_1' \mathbf{r}_2' \rangle \left[-\nabla_1 + \nabla_1' + \nabla_2 + \nabla_2' \right] A(\mathbf{r}_2' \mathbf{r}_2) A(\mathbf{r}_1'' \mathbf{r}_1) \\ & (4.115) \end{aligned}$$

(where the energy variables and integrations have been omitted).

If we introduce the change of variables

$$\begin{aligned} r_1 &= R & r_1'' &= R - r \\ r_2 &= R' - r' & r_2' &= R' \end{aligned} \quad (4.116)$$

then the integral of the potential contribution over a macroscopic region V may be written as

$$\begin{aligned} \int_V (dR) \nabla \cdot T^{(1)}(R) &= \int (dR')(dr)(dr') \int_V (dR) \langle R, R' - r' | T | R - r, R' \rangle \\ &\times [-\nabla_R + \nabla_{R'} - 2 \nabla_r] A(R', R' - r') A(R - r, R) \quad (4.117) \end{aligned}$$

Then, by using a second change of variables,

$$\begin{aligned} \bar{R} &= R - r & \bar{R}' &= R' - r' \\ \bar{r} &= -r & \bar{r}' &= -r' \end{aligned} \quad (4.118)$$

and again employing the symmetry of T and A , we obtain

$$\begin{aligned} \int_V (dR) \nabla \cdot T^{(1)}(R) &= \int (d\bar{R}')(d\bar{r})(d\bar{r}') \int_{V'} (d\bar{R}) \langle \bar{R}, \bar{R}' - \bar{r}' | T | \bar{R} - \bar{r}, \bar{R}' \rangle \\ &\times [\nabla_{\bar{R}} + \nabla_{\bar{R}'} + 2 \nabla_{\bar{r}}] A(\bar{R}', \bar{R}' - \bar{r}') A(\bar{R} - \bar{r}, \bar{R}) \quad (4.119) \end{aligned}$$

where V' is the region of \bar{R} such that $\bar{R} - \bar{r}$ is in V . By averaging (4.117) and (4.119) we may write the integral as two terms:

$$\int_V (dR) \nabla \cdot T^{(1)}(R) = I + I' \quad (4.120)$$

which are

$$I = \int (dR')(dr)(dr') \int_V (dR) \langle R, R' - r' | T | R - r, R' \rangle \nabla_{R'} A(R', R' - r') A(R - r, R) \quad (4.121)$$

and

$$\begin{aligned} I' &= \frac{1}{2} \int (dR')(dr)(dr') \int_{V' - V} (dR) \langle R, R' - r' | T | R - r, R' \rangle \\ &[\nabla_R + \nabla_{R'} + 2 \nabla_r] A(R', R' - r') A(R - r, R) \quad (4.122) \end{aligned}$$

Now consider I. Using partial integration and the fact that $\nabla_R T = -\nabla_{R'} T$, we may write this integral as

$$I = \int (dr)(dr') \int_V (dR) A(R, R' - r') A(R - r, R) \frac{1}{2} [\nabla_R - \nabla_{R'}] < R, R' - r' | T | R - r, R' > . \quad (4.123)$$

In this form the integrand is antisymmetric under the interchanges $R \leftrightarrow R'$ and $r \leftrightarrow r'$, so that the portion of the integral which arises from R' in V vanishes, and we may limit R' to the region outside V . Then, since the integrand vanishes when $R - R'$ is macroscopically large, we find that R and R' are limited to a region near the surface of V . For a portion of this region where the system has local uniformity we may write the integration as

$$\int_{\text{non-V}} (dR') \int_V (dR) = - \int dS n \cdot \int (R - R') d(R - R') \begin{cases} 1 & ; n \cdot (R - R') < 0 \\ 0 & ; n \cdot (R - R') > 0 \end{cases} , \quad (4.124)$$

where S is the surface of V and n is a unit vector normal to the surface in the outward direction. Thus, using the antisymmetry of the integrand, we have

$$I = \int dS n \cdot \left\{ -\frac{1}{2} \int d(R - R') (dr)(dr') (R - R') A(R', R' - r') A(R - r, R) \frac{1}{2} [\nabla_R - \nabla_{R'}] < R, R' - r' | T | R - r, R' > \right\} , \quad (4.125)$$

where the quantity in brackets is identified as the I-contribution to $T^{(1)}(R)$.

Next, consider I' . In this case, the vanishing of the integrand for macroscopically large r limits the integration over $V' - V$ to a region near the surface of V , and for a locally uniform portion of this region we have

$$\int_{V' - V} (dR) = \int dS n \cdot r , \quad (4.126)$$

so that

$$I' = \int dS n \cdot \left\{ \frac{1}{2} \int (dR')(dr)(dr') r < R, R' - r' | T | R - r, R' > [\nabla_R + \nabla_{R'} + 2\nabla_r] A(R', R' - r') A(R - r, R) \right\} , \quad (4.127)$$

where the quantity in brackets is the I' -contribution to $T^{(1)}(R)$.

For a homogeneous system (or within a locally uniform region), A will depend only upon the difference of its spatial coordinates, so that the gradients ∇_R and $\nabla_{R'}$ in the I' -contribution will vanish. Then, by using partial integration on the I' -contribution, we may write the combined contribution as

$$T^{(1)} = -\frac{1}{2} \int_{-\infty}^{\mu} \frac{d\omega d\omega'}{(2\pi)^2} \int d(R-R') (dr)(dr') A(-r, \omega) A(r', \omega')$$

$$\left[\frac{1}{2} (R-R') (\nabla_R - \nabla_{R'}) + 2 \nabla_{\mathbf{r}} \mathbf{r} \right] \times \langle R, R' - \mathbf{r} | T(\omega + \omega') | R - \mathbf{r}, R' \rangle, \quad (4.128)$$

which becomes in momentum space (where δ is the unit tensor)

$$T^{(1)} = \frac{1}{2} \int_{-\infty}^{\mu} \frac{d\omega d\omega'}{(2\pi)^2} \int \frac{(dp)(dp')}{(2\pi)^3} A(p, \omega) A(p', \omega')$$

$$[\delta + 2p \nabla_p] \left\langle \frac{p - p'}{2} \right| t_{\text{sym}} \left(\omega + \omega' - \frac{(p + p')^2}{4m} \right) \left| \frac{p - p'}{2} \right\rangle. \quad (4.129)$$

The substitution of equations (4.80) and (4.77) reduces this to

$$T^{(1)} = \frac{1}{2} \delta \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \int \frac{(dp)}{(2\pi)^3} A(p, \omega) \left[1 + \frac{2}{3} p \frac{\partial}{\partial p} \right] V(p, \omega)$$

$$= \frac{1}{2} \delta \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \rho(p) \left[1 + \frac{2}{3} p \frac{\partial}{\partial p} \right] V(p, h(p)) \quad (4.130)$$

Now, the partial derivative of $V(p, h(p))$ may be related to the total derivative of $V(p)$ by

$$\frac{\partial}{\partial p} V(p, h(p)) = \frac{d}{dp} V(p, h(p)) - \frac{\partial}{\partial \omega} V(p, h(p)) \frac{d}{dp} h(p)$$

$$= \frac{d}{dp} V(p) - \left[1 - \rho^{-1}(p) \right] \left[\frac{p}{m} + \frac{d}{dp} V(p) \right] \quad (4.131)$$

Substitution of this result into (4.130) and integration by parts gives

$$T^{(1)} = \delta \left\{ \frac{p_f^3}{6\pi^2} V(p_f) + \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \left[\frac{2}{3} (1 - \rho(p)) \frac{p^2}{2m} + \left(\frac{1}{2} \rho(p) - 1 \right) V(p) \right] \right\} \quad (4.132)$$

On the other hand, the kinetic portion of the stress tensor (4.112) for a homogeneous system is given in momentum space by

$$T^{(0)} = \frac{2}{3} \delta \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \int \frac{(dp)}{(2\pi)^3} \frac{p^2}{2m} A(p, \omega) = \frac{2}{3} \delta \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \frac{p^2}{2m} \rho(p) \quad (4.133)$$

The pressure is then given by the average diagonal element of the full stress tensor $T^{(0)} + T^{(1)}$:

$$p = \frac{p_f^5}{30\pi^2 m} + \frac{p_f^3}{6\pi^2} V(p_f) + \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} \left[\frac{1}{2} \rho(p) - 1 \right] V(p) \quad (4.134)$$

It is this expression, which we will call the L-T (local transport) pressure, which must be used to obtain the zero point in the homogeneous-case computation which provides the boundary conditions for the inhomogeneous case.⁽¹⁵⁾

A computation of the μ -pressure and the L-T pressure was included in the computer program described in the last section. The numerical results for these pressures are included in Appendix B and are shown in Figure 9, along with the F-W pressure, which was obtained by hand computation. It can be seen that the three pressure relations lead to different, but similarly behaved, functions, with $P_\mu < P_{L-T} < P_{F-W}$.

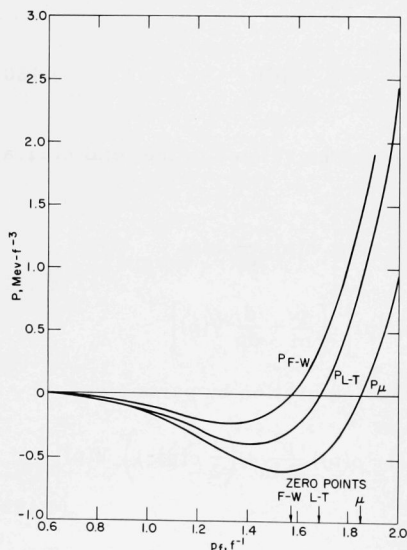


Fig. 9

Pressure P as a function of the Fermi momentum p_f for homogeneous nuclear matter in the Puff-Martin approximation, using Eqs. (4.102)(F-W), (4.103)(μ), and (4.134)(L-T). These functions must be multiplied by a degeneracy factor of 4.

The computer program was then iterated (using a method described in Appendix A) to produce the values of p_f and the various nuclear parameters at the μ and L-T zero points. The functions $V(p)$ and $\rho(p)$ at these zero points are shown in Figure 10 and tabulated in Appendix B. The important nuclear parameters are summarized in Table IV, along with the corresponding parameters for the F-W zero point, which are quoted or calculated from the results of Falk and Wilets.⁽¹⁴⁾

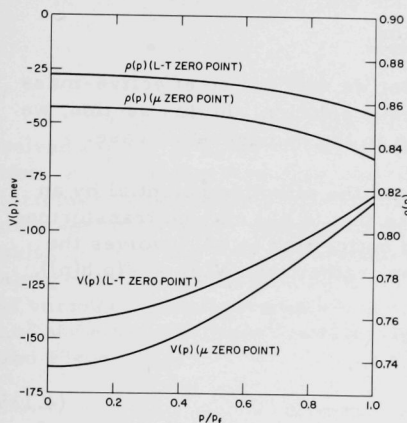


Fig. 10

Effective potential $V(p)$ and momentum distribution $\rho(p)$ as functions of p/p_f for homogeneous nuclear matter in the Puff-Martin approximation, at the μ and local transport (L-T) zero points.

Table IV

PARAMETERS OF HOMOGENEOUS NUCLEAR MATTER IN THE
PUFF-MARTIN APPROXIMATION, USING
VARIOUS ZERO POINTS

	Pressure Expression Set to Zero:		
	$\mu(4.103)$	L-T (4.134)	F-W (4.102) ^a
Fermi momentum p_f , (f^{-1})	1.8491	1.6865	1.575
Chemical potential μ , (Mev)	-14.437	-24.028	-27.7
Density ρ , ^b (f^{-3})	0.09028	0.06991	0.0579
Interparticle spacing r_0 , (f)	0.871	0.949	1.01
Energy density ϵ , ^b (Mev- f^{-3})	-1.3034	-1.1903	-1.01
Energy per particle ϵ/ρ , (Mev)	-14.437	-17.026	-17.5
μ pressure P_μ , ^b (Mev- f^{-3})	0.0	-0.4895	-0.59
L-T pressure P_{L-T} , ^b (Mev- f^{-3})	0.9073	0.0	-0.27 approx
F-W pressure P_{F-W} , ^b (Mev- f^{-3})	1.4 approx	0.38 approx	0.0

^aQuoted or calculated from results given in reference 14.

^bThese quantities must be multiplied by a degeneracy factor of 4.

Unlike the Hartree case, the present approximation (at all three zero points) gives a binding energy per particle and density which are in reasonable agreement with experimental results. It is probable that this agreement does not imply a similar accuracy in $V(p)$ and $\rho(p)$, but the results are at least a qualitatively valid description of nuclear matter, and indicate that a repulsive core in the interparticle potential is probably the primary agent in causing saturation.

IV.4 - The Effective-mass Approximation

Just as in the Hartree-Fock case, we will use an effective-mass approximation to obtain the inhomogeneous solution. In this section, we investigate the equivalent approximation in the homogeneous case.

As before, we wish to approximate the effective potential by an even quadratic function of momentum, so that (4.48) may be transformed into a local equation. It is important to notice that (4.48) involves the function $V(p, \omega)$, so that it is this function, rather than $V(p) = V(p, h(p))$, which must be quadratic in p .

Thus, we approximate $V(p, \omega)$ by

$$V_{ap}(p, \omega) = V_0(\omega) + V_2(\omega)p^2 \quad (4.135)$$

The quantities $V_0(\omega)$ and $V_2(\omega)$ may be obtained by the least-squares procedure of equations (2.66) to (2.68). This gives

$$V_{\{0\}}^{(2)}(\omega) = \frac{1}{\pi^{3/2}} \int (dp) e^{-\frac{p^2}{\beta^2}} \left\{ \begin{array}{l} \frac{5}{2} \frac{1}{\beta^3} - \frac{p^2}{\beta^5} \\ - \frac{1}{\beta^5} + \frac{2}{3} \frac{p^2}{\beta^7} \end{array} \right\} V(p, \omega) \quad (4.136)$$

where β is an unspecified parameter of the weight function (2.67). Substitution of (4.83) and (4.82) yields

$$V_{\{0\}}^{(2)}(\omega) = \int_{|p_2| < p_f} (dp_2) K_{\{0\}}^{(2)}(p_2, \omega + h(p_2)) \rho(p_2) \quad (4.137)$$

where

$$K_{\{0\}}^{(2)}(p_2, \omega) = \frac{1}{\pi^{3/2}} \int (dp_1) e^{-\frac{p_1^2}{\beta^2}} \left\{ \begin{array}{l} \frac{5}{2} \frac{1}{\beta^3} - \frac{p_1^2}{\beta^5} \\ - \frac{1}{\beta^5} + \frac{2}{3} \frac{p_1^2}{\beta^7} \end{array} \right\} \\ \times < \frac{p_1 - p_2}{2} \left| t_{\text{sym}} \left(\omega - \frac{(p_1 + p_2)^2}{4m} \right) \right| \frac{p_1 - p_2}{2} > \quad (4.138)$$

Thus, the replacement of $V(p, \omega)$ by $V_0(\omega) + V_2(\omega)p^2$ may be carried out by replacing (4.82) by

$$\begin{aligned}
 K(p_1 p_2, \omega) &= K_0(p_2, \omega) + K_2(p_2, \omega)p_1^2 \\
 &= \frac{1}{\pi^{3/2}} \int (dp_3) e^{-\frac{p_3^2}{\beta^2}} \left[\frac{5}{2} \frac{1}{\beta^3} - \frac{p_3^2}{\beta^5} - \frac{p_1^2}{\beta^5} + \frac{2}{3} \frac{p_1^2 p_3^2}{\beta^7} \right] \\
 &\times \left\langle \frac{p_3 - p_2}{2} \right| t_{\text{sym}} \left(\omega - \frac{(p_3 + p_2)^2}{4m} \right) \left| \frac{p_3 - p_2}{2} \right\rangle. \quad (4.139)
 \end{aligned}$$

The resulting equations for the effective-mass approximation were solved for the L-T zero point in the manner described in the previous section. As in the Hartree case, the value of the weight parameter β was determined by the requirement that the computed value of p_f equal the value obtained in the exact case. This led to a value of $\beta = 0.8931 \text{ f}^{-1}$. The results for $V(p)$ and $\rho(p)$ are tabulated in Appendix B and shown in Figure 11, along with the corresponding exact solutions. Table V gives a comparison of various nuclear parameters for the effective-mass and exact solutions, and the effective-mass functions $V_0(\omega)$ and $V_2(\omega)$ are given in Table VI and Figure 12.

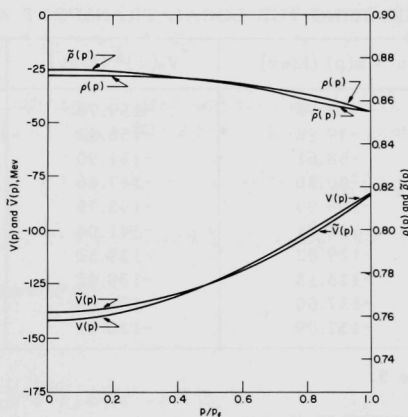


Fig. 11. Effective potential $V(p)$ and momentum distribution $\rho(p)$ as functions of p/p_f for homogeneous nuclear matter in the Puff-Martin approximation, with and without the effective-mass approximation. In both cases the local-transport zero point is used. The effective-mass functions are indicated by a tilde.

Table V

PARAMETERS OF HOMOGENEOUS NUCLEAR MATTER IN THE
PUFF-MARTIN APPROXIMATION, USING THE LOCAL-
TRANSPORT ZERO POINT, FOR THE EXACT AND
EFFECTIVE-MASS SOLUTIONS

	Exact	Eff. Mass
Fermi momentum p_f , (f^{-1})	1.6865	1.6865
Chemical potential μ , (Mev)	-24.028	-24.766
Density ρ , ^a (f^{-3})	0.06991	0.06982
Interparticle spacing r_0 , (f)	0.949	0.949
Energy density ϵ , ^a (Mev- f^{-3})	-1.1903	-1.2323
Energy per particle ϵ/ρ , (Mev)	-17.026	-17.649
μ pressure P_μ , ^a (Mev- f^{-3})	-0.4895	-0.4969
L-T pressure P_{L-T} , ^a (Mev- f^{-3})	0.0	0.0

^aThese quantities must be multiplied by a degeneracy factor of 4.

Table VI

ENERGY-DEPENDENT COEFFICIENTS OF THE EFFECTIVE-MASS
APPROXIMATION FOR THE EFFECTIVE POTENTIAL, IN THE
PUFF-MARTIN APPROXIMATION FOR HOMOGENEOUS
MATTER, USING THE LOCAL-TRANSPORT ZERO POINT

p (f^{-1})	$\omega = h(p)$ (Mev)	$V_0(\omega)$ ^a (Mev)	$V_2(\omega)$ ^a (Mev- f^2)
1.6645	-27.78	-159.78	26.91
1.5727	-39.82	-156.42	26.41
1.4161	-58.61	-151.90	25.78
1.2087	-80.30	-147.46	25.23
0.9688	-100.99	-143.75	24.83
0.7177	-117.71	-141.04	24.55
0.4778	-129.02	-139.32	24.39
0.2703	-135.13	-138.42	24.31
0.1138	-137.50	-138.08	24.28
0.0220	-137.99	-138.01	24.27

^aSee footnote 5.

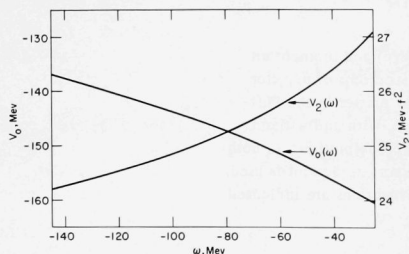


Fig. 12

The coefficients of the effective-mass approximation for the energy-dependent effective potential of homogeneous nuclear matter in the Puff-Martin approximation (at the local-transport zero point). The constant term $V_0(\omega)$ and the quadratic term $V_2(\omega)$ are given as functions of ω (see footnote 5).

IV.5 - The Density Correlation Function

Once the basic functions $V(p)$ and $\rho(p)$ have been obtained for homogeneous matter, a wide variety of nuclear properties may be computed. We will obtain results for one such property, the density correlation function, in order to reveal the characteristics of nuclear correlations in the Puff-Martin approximation. The density correlation function $f(r_1 \zeta_1, r_2 \zeta_2)$ measures the probability of simultaneously finding a particle at r_1 with spin and isospin ζ_1 , and a second particle at r_2 with spin and isospin ζ_2 . The function may be expressed in terms of G_2 as

$$f(r_1 \zeta_1, r_2 \zeta_2) = - G_2(r_1 \zeta_1 t \ r_2 \zeta_2 t; r_1 \zeta_1 t^+ \ r_2 \zeta_2 t^+) \quad (4.140)$$

The dependence on internal variables is as follows; let j be the spin coordinate and k the isospin coordinate. Then

$$G_2 = \begin{cases} G_{tt} & ; & j_1 = j_2, \quad k_1 = k_2 \\ \frac{1}{2} (G_{st} + G_{tt}) & ; & j_1 \neq j_2, \quad k_1 = k_2 \\ \frac{1}{2} (G_{ts} + G_{tt}) & ; & j_1 = j_2, \quad k_1 \neq k_2 \\ \frac{1}{4} (G_{ss} + G_{ts} + G_{st} + G_{tt}) & ; & j_1 \neq j_2, \quad k_1 \neq k_2 \end{cases} \quad (4.141)$$

where the subscripts indicate singlet and triplet matrix elements of G_2 . We also note that if $\bar{X}(1 \ 2 \ 1' \ 2') = X(1 \ 2 \ 2' \ 1')$, then the matrix elements obey

$$\begin{aligned} \bar{X}_{ss}(1 \ 2 \ 1' \ 2') &= X_{ss}(1 \ 2 \ 2' \ 1') & \bar{X}_{st}(1 \ 2 \ 1' \ 2') &= -X_{st}(1 \ 2 \ 2' \ 1') \\ \bar{X}_{ts}(1 \ 2 \ 1' \ 2') &= -X_{ts}(1 \ 2 \ 2' \ 1') & \bar{X}_{tt}(1 \ 2 \ 1' \ 2') &= X_{tt}(1 \ 2 \ 2' \ 1') \end{aligned} \quad (4.142)$$

Thus, equation (4.10) becomes

$$G_2(1 \ 2; 1' \ 2') =$$

$$\int [d1''] [d2''] \Omega(1 \ 2; 1'' \ 2'') [G_1(1''; 1') G_1(2''; 2') - \epsilon G_1(1''; 2') G_1(2''; 1')] \quad (4.143)$$

where ϵ is 1 for ss or tt -functions and -1 for ts or st -functions. Then, using (4.12), we get

$$\begin{aligned} G_2(r_1 t \ r_2 t; r_1 t^+ r_2 t^+) &= \int (dr_1'') (dr_2'') \int_0^T dt'' \Omega(r_1 r_2 t; r_1'' r_2'' t'') \\ &\times [G_1(r_1'' t''; r_1 t^+) G_1(r_2'' t''; r_2 t^+) - \epsilon G_1(r_1'' t''; r_2 t^+) G_1(r_2'' t''; r_1 t^+)] \quad (4.144) \end{aligned}$$

By performing the usual transformation to an energy representation we may obtain

$$f(r_1 - r_2) = \rho^2 - \epsilon \left\{ \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(r_1 r_2 \omega) \right\}^2 - \int_{-\infty}^{2\mu} \frac{d\omega}{2\pi} \frac{1}{i} [C(r_1 r_2 \omega - i\epsilon) - C(r_1 r_2 \omega + i\epsilon)], \quad (4.145)$$

where

$$C(r_1 r_2 \omega) = \int (dr'_1)(dr'_2)(dr''_1)(dr''_2) \Lambda^\circ(r_1 r_2 r'_1 r'_2 \omega) \langle r'_1 r'_2 | T(\omega) | r''_1 r''_2 \rangle \Lambda(r''_1 r''_2 r_1 r_2 \omega), \quad (4.146)$$

where T is formed from a symmetrized or antisymmetrized combination of scattering matrices for the appropriate spin-isospin state, and

$$\Lambda(r_1 r_2 r'_1 r'_2 \omega) = \int \frac{d\omega_1 d\omega_2}{(2\pi)^2} \frac{A(r_1 r'_1 \omega_1) A(r_2 r'_2 \omega_2)}{\omega - \omega_1 - \omega_2} \left\{ \frac{1}{2} \tanh \frac{i\tau}{2} (\omega_1 - \mu) + \frac{1}{2} \tanh \frac{i\tau}{2} (\omega_2 - \mu) \right\}, \quad (4.147)$$

and similarly for Λ° . However, since in the low-temperature limit Λ° and T are continuous for $\omega < 2\mu$, the effect of taking the discontinuity of C across the real axis is simply to replace Λ by the corresponding spectral function, which is (at zero temperature)

$$\int_{\mu - \frac{\omega}{2}}^{\frac{\omega}{2} - \mu} \frac{d\omega'}{2\pi} A(r_1 r'_1, \frac{\omega}{2} + \omega') A(r_2 r'_2, \frac{\omega}{2} - \omega') \quad (4.148)$$

By transforming into momentum space we may reduce f to

$$f(r) = \rho^2 - \epsilon \left\{ \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot r} A(p, \omega) \right\}^2 + \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot r} \int \frac{(dp_1)(dp_2)}{(2\pi)^3} \int_{-\infty}^{\mu} \frac{d\omega_1 d\omega_2}{(2\pi)^2} \frac{\langle p + \frac{p_1 - p_2}{2} | \tilde{t}(\omega_1 + \omega_2 - \frac{(p_1 + p_2)^2}{4m}) | \frac{p_1 - p_2}{2} \rangle}{\omega_1 + \omega_2 - \frac{1}{2m} (p_1 + p)^2 - \frac{1}{2m} (p_2 - p)^2} A(p_1 \omega_1) A(p_2 \omega_2) \quad (4.149)$$

where

$$\langle p|\tilde{t}|p'\rangle = \langle p|t|p'\rangle - \epsilon \langle p|t|-p'\rangle \quad (4.150)$$

The substitution of (4.77) reduces this to

$$f(r) = \rho^2 - \epsilon \left\{ \int_{|p| < p_f} \frac{(dp)}{(2\pi)^3} e^{ip \cdot r} \rho(p) \right\}^2 + \int \frac{(dp)}{(2\pi)^3} e^{ip \cdot r} \int_{|p_1|, |p_2| < p_f} \frac{(dp_1)(dp_2)}{(2\pi)^3} \frac{\langle p + \frac{p_1 - p_2}{2} | \tilde{t} \left(V(p_1) + V(p_2) + \frac{(p_1 - p_2)^2}{4m} \right) | \frac{p_1 - p_2}{2} \rangle}{V(p_1) + V(p_2) - \frac{1}{m} p \cdot (p_1 - p_2 + p)} \rho(p_1) \rho(p_2) \quad (4.151)$$

Now consider the various combinations (4.141) of matrix elements which appear in f . For our particular choice of a potential, which satisfies (4.94) and $\langle p|t|p'\rangle = \langle p|t|-p'\rangle$, the dependence of f on internal variables is considerably simplified. The second term in (4.151), which describes exclusion effects, vanishes for unlike particles, whereas the third term vanishes for identical particles, which are excluded from the S-state and do not interact. For unlike particles, the combinations of the singlet and triplet scattering matrices which form \tilde{t} are

<u>spin</u>	<u>isospin</u>	
opposite	same	$\tilde{t} = t_s$
same	opposite	$\tilde{t} = t_t$
opposite	opposite	$\tilde{t} = 1/2 (t_s + t_t)$

(4.152)

The four correlation functions, as calculated for the local-transport zero point (without the effective-mass approximation) are tabulated in Table VII. They are also shown in Figure 13, along with the function

$$N(r) = \frac{1}{\rho} \int_{|r'| < r} (dr') \sum_{\xi} f(r' \xi) \quad (4.153)$$

which gives the expected number of additional particles to be found within the distance r of a given particle. It can be seen that there is only a 24% probability of finding an additional particle within 0.7 fermi, which is the approximate distance at which correlation effects other than the exclusion principle begin to play a major role. In view of this result, it can be expected that correlations of more than two particles should be sufficiently rare as to have only slight effects on nuclear properties.

Table VII

DENSITY CORRELATION FUNCTION FOR HOMOGENEOUS MATTER IN THE PUFF-MARTIN APPROXIMATION, USING THE LOCAL-TRANSPORT ZERO POINT

r (fermi)	Correlation Function (fermi ⁻⁶) for:				
	spin:	same	opposite	same	opposite
	isospin:	same	same	opposite	opposite
0.0	J	0.011229	0.023994	0.017612	
0.1		0.000028	0.008197	0.017014	0.012605
0.2		0.000110	0.005577	0.011210	0.008393
0.3		0.000244	0.003280	0.006326	0.004803
0.4		0.000427	0.001228	0.002151	0.001689
0.45 ^a		0.000535	0.000272	0.000272	0.000272
0.5		0.000653	0.001733	0.002138	0.001936
0.6		0.000915	0.003545	0.004315	0.003930
0.7		0.001208	0.004495	0.005329	0.004912
0.8		0.001522	0.004985	0.005755	0.005370
0.9		0.001851	0.005220	0.005882	0.005551
1.0		0.002185	0.005315	0.005858	0.005586
1.2		0.002843	0.005309	0.005646	0.005478
1.5		0.003708	0.005166	0.005311	0.005239
2.0		0.004605	0.004986	0.005012	0.004999
2.5		0.004877	0.004915	0.004917	0.004916
3.0		0.004869	0.004894	0.004893	0.004893
3.5		0.004852	0.004888	0.004888	0.004888
4.0		0.004873	0.004887	0.004887	0.004887
4.5		0.004887	0.004887	0.004887	0.004887

^aShell radius.

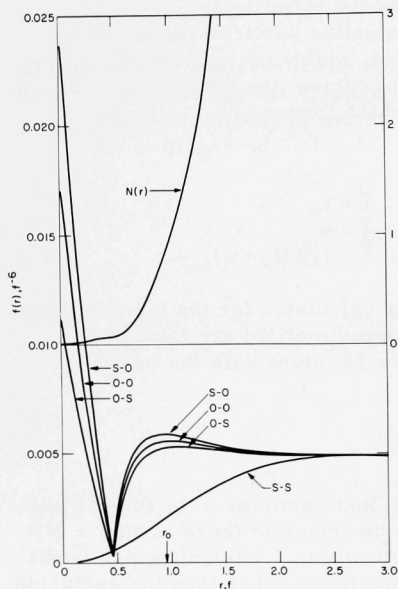


Fig. 13

Density correlation function $f(r)$ and its integral $N(r)$ as functions of the distance r , for homogeneous nuclear matter in the Puff-Martin approximation (at the local-transport zero point). The density correlation function is given for particles with the same spin and isospin (S-S), opposite spin and same isospin (O-S), same spin and opposite isospin (S-O), and opposite spin and isospin (O-O). The function $N(r)$ [cf. Eq. (4.153)] is the expected number of additional particles within a radius r of a given particle. Note that $f(r)$ and $N(r)$ have ordinates with different origins.

A rather disturbing result is the large value of the unlike-particle correlation functions within the core radius of 0.45 fermi. This is a consequence of our use of a hard shell to approximate a hard core, and represents the unphysical situation of particles bound inside the shell. However, the large value of the correlation functions is offset by the small size of the shell, so that $N(r)$ is only 6.3% at the shell radius.

CHAPTER V

THE PUFF-MARTIN APPROXIMATION IN THE INHOMOGENEOUS CASE

V.1. The Wave-function Expansion Method

In this chapter we derive the inhomogeneous equations for the Puff-Martin approximation and describe their numerical solution. Because of its breakdown in the Hartree case, we omit any investigation of the Thomas-Fermi approach and turn directly to the expansion of the spectral function in a set of wave functions.

The wave-function expansion of A , along with the appropriate wave equation and normalization conditions, was derived in Section III.2 for a generalized energy-dependent potential of the form which occurs in equation (4.49). As a result, these derivations are correct for the Puff-Martin as well as the Hartree-Fock approximations, and we may use equations (3.16) to (3.50) without modification. In particular, we note that (3.32), (3.34), and (3.35) correctly anticipate the definitions of the homogeneous-case functions $h(p)$, $A_{\text{hom}}(p)$, and $\rho(p)$ given by (4.75), (4.77), and (4.78).

The remaining task is the derivation of expressions for the density, energy density, and effective potential in terms of the partially transformed spectral function $A(p_{\mathbf{r}} z z' \omega)$. As in the Hartree approximation, the density may be obtained by substituting (3.24) into (2.29). The resulting equation,

$$\rho(Z) = \int_0^{\text{Pf}} \frac{p_{\mathbf{r}} dp_{\mathbf{r}}}{2\pi} \int_{h(p_{\mathbf{r}}) - (p_{\mathbf{r}}^2/2m)}^{\mu - (p_{\mathbf{r}}^2/2m)} \frac{d\omega}{2\pi} A(p_{\mathbf{r}} Z Z \omega) \quad , \quad (5.1)$$

is similar to (3.51) except for the more complicated lower limit of the ω -integration. Similarly, by substituting (3.24) into (2.33), we obtain the energy density

$$\epsilon(Z) = \frac{1}{2} \int_0^{\text{Pf}} \frac{p_{\mathbf{r}} dp_{\mathbf{r}}}{2\pi} \int_{h(p_{\mathbf{r}}) - (p_{\mathbf{r}}^2/2m)}^{\mu - (p_{\mathbf{r}}^2/2m)} \frac{d\omega}{2\pi} \lim_{Z' \rightarrow Z} \left[\omega + \frac{2p_{\mathbf{r}}^2}{2m} - \frac{1}{2m} \frac{\partial^2}{\partial Z^2} \right] A(p_{\mathbf{r}} Z Z' \omega) \quad . \quad (5.2)$$

The effective potential $V(R p \omega)$ is defined by the energy-dependent generalization of (3.7):

$$V\left(R + \frac{\mathbf{r}}{2}, R - \frac{\mathbf{r}}{2}, \omega\right) = \int \frac{(dp)}{(2\pi)^3} e^{i\mathbf{p} \cdot \mathbf{r}} V(R p \omega) \quad . \quad (5.3)$$

Substitution of (4.58) and (3.24) into the inverse of (5.3) gives

$$\begin{aligned}
 V(Z_1 p_1 \omega) = & \int (dR_2) \frac{(dp_2)}{(2\pi)^3} \int^\mu \frac{d\omega'}{2\pi} \\
 & \times \left\{ \int (dr) e^{-\frac{i}{2}(p_1 - p_2) \cdot r} \left\langle R_1 - R_2 + \frac{r}{2} \right| t_{\text{sym}} \left(\omega + \omega' - \frac{(p_1 + p_2)^2}{4m} \right) \right| R_1 - R_2 - \frac{r}{2} \rangle \right\} \\
 & \times \int dz_2 e^{-ip_{z2} z_2} A \left(p_{r2}, Z_2 + \frac{z_2}{2}, Z_2 - \frac{z_2}{2}, \omega' - \frac{p_{r2}^2}{2m} \right)
 \end{aligned} \quad (5.4)$$

As before, to carry out the effective-mass approximation we must fit (5.4) to a quadratic function of the form (3.41) by the method of least squares. The procedure of equations (3.54) to (3.57) is still applicable, and it yields

$$V_i(Z\omega) = \sum_j M_{ij} U_j(Z\omega) \quad , \quad (5.5)$$

where M_{ij} is given by (3.57) and

$$\begin{aligned}
 U_{\begin{Bmatrix} 0 \\ 1 \\ 11 \end{Bmatrix}}(Z_1 \omega) = & \int (dR_2) dz_2 \frac{dp_{x2} dp_{y2}}{(2\pi)^2} \int^\mu \frac{d\omega'}{2\pi} \\
 & \left\{ \frac{1}{\beta^3 \pi^{3/2}} \int (dp_1) e^{-p_1^2/\beta^2} \begin{Bmatrix} 1 \\ p_{1r}^2 \\ p_{1z}^2 \end{Bmatrix} \times \int \frac{dp_{z2}}{2\pi} e^{-ip_{z2} z_2} \int (dr) e^{-\frac{i}{2}(p_1 - p_2) \cdot r} \right. \\
 & \left. \left\langle R_1 - R_2 + \frac{r}{2} \right| t_{\text{sym}} \left(\omega + \omega' - \frac{(p_1 + p_2)^2}{4m} \right) \right| R_1 - R_2 - \frac{r}{2} \rangle \right\} \\
 & \times A \left(p_{r2}, Z_2 + \frac{z_2}{2}, Z_2 - \frac{z_2}{2}, \omega' - \frac{p_{r2}^2}{2m} \right) \quad ,
 \end{aligned} \quad (5.6)$$

and β is the matching parameter obtained in the homogeneous case.

Now (5.6) expresses three functions of two variables as fourfold multiple integrals of a kernel function times the spectral function A . Unfortunately, even on a high-speed computer such as the IBM 704, the direct numerical evaluation of this equation during each iteration of a self-consistent computation would require a total of 40 to 80 hr of machine time. To circumvent this difficulty we have used the artifice of approximating the scattering matrix by a sum of exponential functions of energy. This approximation allows (5.6) to be simplified considerably and results in nearly a twentyfold reduction in computing time.

Specifically, using (4.95) and (4.96) we may express the scattering matrix as

$$t_{\text{sym}} = \frac{3}{4m\pi} [\theta_{yy \text{ sing}}(\omega)\tau_{yy \text{ sing}} + \theta_{yy \text{ trip}}(\omega)\tau_{yy \text{ trip}} + \theta_{yc \text{ sing}}(\omega)\tau_{yc \text{ sing}} + \theta_{yc \text{ trip}}(\omega)\tau_{yc \text{ trip}} + \theta_{cc}(\omega)\tau_{cc}] , \quad (5.7)$$

where the combination $\theta_{cc} = \theta_{cc \text{ sing}} + \theta_{cc \text{ trip}}$ may be used, since τ_{cc} is independent of the spin state. We approximate the five theta functions by

$$\theta_k(\omega) \approx \sum_{L=1}^7 C_{kL} e^{\alpha_L \omega} . \quad (5.8)$$

To determine the parameters in (5.8), let us choose the α_L 's arbitrarily and determine the C 's by the method of least squares. We minimize the quantities

$$\xi_k = \int_{\omega_0}^{\omega_1} d\omega \left[\theta_k(\omega) - \sum_{L=1}^7 C_{kL} e^{\alpha_L \omega} \right]^2 , \quad (5.9)$$

where the θ 's are given by (4.99) and (4.100). This leads to the result

$$C_{kL} = \sum_{m=1}^7 V_{km} T_{mL}^{-1} , \quad (5.10)$$

where

$$V_{km} = \int_{\omega_0}^{\omega_1} d\omega e^{\alpha_m \omega} \theta_k(\omega) , \quad (5.11)$$

and T^{-1} is the inverse of the matrix T with elements

$$T_{mL} = \int_{\omega_0}^{\omega_1} d\omega e^{(\alpha_m + \alpha_L)\omega} = \frac{1}{\alpha_m + \alpha_L} \left[e^{(\alpha_m + \alpha_L)\omega_1} - e^{(\alpha_m + \alpha_L)\omega_0} \right] . \quad (5.12)$$

The IBM 704 was used to calculate the coefficients C_{kL} by this procedure. The region of matching was chosen to be $\omega_0 = -500$ Mev to $\omega_1 = -30$ Mev. The chosen α_L 's and the calculated C 's are given in Table VIII.

Table VIII

PARAMETERS OF EXPONENTIAL APPROXIMATION
FOR THE SCATTERING MATRIX^a

L	$\alpha_L(\text{Mev}^{-1})$	$C_{yyS}(f^{-3})$	$C_{yyt}(f^{-3})$	$C_{yCS}(f^{-2})$	$C_{yct}(f^{-2})$	$C_{CC}(f^{-1})$
1	0	-45.911	-139.633	6.7168	16.8971	6.6573
2	1/320	-22.324	-136.417	11.3835	38.067	-24.531
3	1/160	5.2630	18.7878	-4.1329	-7.6052	13.1313
4	1/80	-19.0556	-114.409	8.1311	29.783	-16.0706
5	1/40	-12.6734	-126.036	3.6526	28.581	-4.4934
6	1/20	-25.249	-215.04	9.1383	52.000	-18.2438
7	1/10	-32.711	-550.95	10.4509	128.249	-30.512

^aSee equations (5.7) and (5.8).

In order to estimate the accuracy of this approximation, a table of the exact and approximate theta functions, and the absolute and relative errors, was computed for values of ω from -500 Mev to -30 Mev at intervals of about 10 Mev. For the functions $\theta_{yy \text{ sing}}$, $\theta_{yy \text{ trip}}$, $\theta_{yc \text{ sing}}$, and $\theta_{yc \text{ trip}}$, the largest relative error was less than 0.08 per cent. Since θ_{CC} has a zero in the matching region, its maximum relative error was infinite, but the largest absolute error in the interval was less than one per cent of its value at -500 Mev and 0.1 per cent of its value at -30 Mev.

An attempt was made to improve the approximation by optimizing the choice of the exponents α_L by means of Prony's method. However, the method failed to give consistent results, presumably because large variations in the α_L 's had little effect on the accuracy of the matching. (Mathematically, this would lead to the inversion of a nearly singular matrix.)

To apply this exponential approximation to our expressions for V, we substitute (5.7) and (5.8) into (5.5) and (5.6), obtaining

$$\begin{aligned}
 \left\{ \begin{array}{c} 0 \\ \perp \\ \parallel \end{array} \right\}^{(Z_1, \omega)} &= \sum_{L=1}^7 e^{\alpha_L \omega} \int_0^\infty \frac{p_{r2} dp_{r2}}{2\pi} \int dZ_2 dz_2 K_L \left\{ \begin{array}{c} 0 \\ \perp \\ \parallel \end{array} \right\}^{(Z_2 z_2 p_{r2})} \\
 &\times \int^\mu \frac{d\omega'}{2\pi} e^{\alpha_L \omega'} A \left(p_{r2}, Z_1 + Z_2 + \frac{z_2}{2}, Z_1 + Z_2 - \frac{z_2}{2}, \omega' - \frac{p_{r2}^2}{2m} \right),
 \end{aligned}
 \tag{5.13}$$

where

$$\begin{aligned}
K_L \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\} (Z, z_2 p_{r2}) &= \frac{3}{4m\beta^3\pi^{5/2}} \int dX dY \int (dp_1) e^{-p_1^2/\beta^2} \left\{ \begin{array}{l} 5/2 - p_{1r}^2/\beta^2 - p_{1z}^2/\beta^2 \\ - 1/\beta^2 + p_{1r}^2/\beta^4 \\ - 1/\beta^2 + 2p_{1z}^2/\beta^4 \end{array} \right\} \\
&\times \int \frac{dp_{zz}}{2\pi} e^{-ip_{zz}z_2} \int (dr) e^{-\frac{i}{2}(p_1 - p_2) \cdot r} \sum_k C_{kL} e^{-\frac{\alpha_L}{4m}(p_1 + p_2)^2} \\
&< R + \frac{r}{2} \left| \tau_k \right| R - \frac{r}{2} > , \quad (5.14)
\end{aligned}$$

and the index k ranges over the five subscripts of the θ 's and the τ 's. To clarify the process of computation, we expand (5.13) into several steps:

$$V \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\} (Z, \omega) = \sum_{L=1}^7 e^{\alpha_L \omega} Q \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\}_L (Z) , \quad (5.15)$$

where

$$Q \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\}_L (Z) = \int_0^{P_f} \frac{p_r dp_r}{2\pi} C \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\}_L (Z, p_r) , \quad (5.16)$$

$$C \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\}_L (Z, p_r) = \int dZ' dz K_L \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\} (Z', z, p_r) B_L (Z + Z', z, p_r) , \quad (5.17)$$

and

$$\begin{aligned}
B_L (Z, z, p_r) &= \int_{h(p_r)}^{\mu} \frac{d\omega}{2\pi} e^{\alpha_L \omega} A \left(p_r, Z + \frac{z}{2}, Z - \frac{z}{2}, \omega - \frac{p_r^2}{2m} \right) \\
&= \int_{h(p_r)}^{\mu} \frac{d\omega}{2\pi} e^{\alpha_L \omega} \psi \left(Z + \frac{z}{2}, p_r, \omega - \frac{p_r^2}{2m} \right) \psi \left(Z - \frac{z}{2}, p_r, \omega - \frac{p_r^2}{2m} \right) . \quad (5.18)
\end{aligned}$$

The area of the p_r, ω -integration has been limited to take into account the lower bound in the energy spectrum of the wave functions.

With a little manipulation all but two of the integrations in (5.14) may be performed analytically. The result may be written as

$$K_{Li} (Z, z_2 p_{r2}) = \sum_j M_{ij} \mathcal{K}_{Lj} (Z, z_2 p_{r2}) , \quad (5.19)$$

where

$$\mathcal{K}_L \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\} (Z z_2 P_{R2}) = \frac{1}{\beta^3} e^{-((1/\beta^2) + (\alpha_L/m)) P_{R2}^2} \int_0^\infty p_R dp_R e^{-((1/\beta^2) + (\alpha_L/4m)) P_R^2} \\ \times \left\{ \begin{smallmatrix} I_0(s) \\ (p_{R2}^2 + p_R^2) I_0(s) - 2 p_R P_{R2} I_1(s) \\ I_0(s) \end{smallmatrix} \right\} L_L \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\} (Z z_2 P_R) \Bigg|_s = p_R P_{R2} ((2/\beta^2) + (\alpha_L/m)) \quad , \quad (5.20)$$

and

$$L_L \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\} (Z z_2 P_R) = \frac{6\beta\sqrt{\pi}}{\sqrt{m\alpha_L}} \int dz \left\{ \begin{smallmatrix} 1 \\ 1 \\ (\beta^2/2) - (\beta^4/4)(z_2 - z)^2 \end{smallmatrix} \right\} e^{-(\beta^2/4)(z_2 - z)^2 - (m/\alpha_L)(z_2 - (z/2))^2} \\ \times \sum_k C_{kL} \left\langle \frac{P_R}{2}, Z + \frac{z}{2} \right| \tau_k \left| \frac{P_R}{2}, Z - \frac{z}{2} \right\rangle \quad ; \quad (\text{for } \alpha_L \neq 0) \\ L_L \left\{ \begin{smallmatrix} 0 \\ 1 \\ 1 \end{smallmatrix} \right\} (Z z_2 P_R) = \frac{12\beta\pi}{m} \left\{ \begin{smallmatrix} 1 \\ 1 \\ (\beta^2/2) - (\beta^4/4)(z_2^2) \end{smallmatrix} \right\} e^{-(\beta^2 z_2^2)/4} \sum_k C_{kL} \left\langle \frac{P_R}{2}, Z + z_2 \right| \tau_k \left| \frac{P_R}{2}, Z - z_2 \right\rangle \quad ; \\ (\text{for } \alpha_L = 0) \quad . \quad (5.21)$$

The expression of the form $\langle p_R z | \tau | p_R' z' \rangle$ in (5.21) indicates a two-dimensional Fourier transform:

$$\langle p_R z | \tau | p_R' z' \rangle = \int \frac{dx dy dx' dy'}{(2\pi)^2} e^{-ip_R \cdot r_R} \langle r | \tau | r' \rangle e^{ip_R' \cdot r_R'} \quad . \quad (5.22)$$

This may be evaluated by substituting (4.97). Let

$$\bar{\alpha} = \sqrt{\alpha^2 + p_R^2} \quad ; \quad \bar{\alpha}' = \sqrt{\alpha'^2 + p_R'^2} \quad . \quad (5.23)$$

Then

$$\langle p_R z | \tau_k | p_R' z' \rangle = \begin{cases} (1/\bar{\alpha} \bar{\alpha}') e^{-\bar{\alpha}|z|} e^{-\bar{\alpha}'|z'|} & (yy) \\ (1/\bar{\alpha}) e^{-\bar{\alpha}|z|} J_c(p_R' \sqrt{r_c^2 - z'^2}) + (1/\bar{\alpha}') e^{-\bar{\alpha}'|z'|} J_c(p_R \sqrt{r_c^2 - z^2}) & (yc) \\ J_c(p_R \sqrt{r_c^2 - z^2}) J_c(p_R' \sqrt{r_c^2 - z'^2}) & (cc) \end{cases} \quad , \quad (5.24)$$

where J_c is a Bessel function which is cut off as its argument goes imaginary

$$J_c(p_r \sqrt{r_c^2 - z^2}) = \begin{cases} J_0(p_r \sqrt{r_c^2 - z^2}) & ; \quad z \leq r_c \\ 0 & ; \quad z > r_c \end{cases} \quad (5.25)$$

V.2. Numerical Computation

We now turn to the numerical solution of the inhomogeneous-case equations in the Puff-Martin approximation. These equations may be treated by an iterative procedure similar to that described in Section III.3 for the Hartree case. The major change is the increased complexity of the integrations which produce the effective potential from the wave functions.

For numerical calculation it is necessary to approximate the integration in (5.17) by weighted sum of $B_L(Z z p_r)$ over a set of equally spaced points in Z and z . Appendix A gives the derivation of a set of coefficients Ψ such that

$$\begin{aligned} C \left\{ \begin{smallmatrix} 0 \\ 1 \\ 11 \end{smallmatrix} \right\}_L(Z p_r) &= \int dZ' dz K_L \left\{ \begin{smallmatrix} 0 \\ 1 \\ 11 \end{smallmatrix} \right\}(Z' z p_r) B_L(Z + Z' z p_r) \\ &= \sum_{m_1=0}^{43} \sum_{m_2=0}^{54} \Psi_{m_1 m_2} \left\{ \begin{smallmatrix} 0 \\ 1 \\ 11 \end{smallmatrix} \right\}_L(p_r) \\ &\quad [B_L(Z + m_1 h_1, m_2 h_2, p_r) + B_L(Z - m_1 h_1, m_2 h_2, p_r)] \end{aligned} \quad (5.26)$$

The calculation of the Ψ -coefficients was performed with the IBM 704. In about 10 hr, the machine produced and stored on magnetic tape a table of 273 44 x 55 matrices $\Psi_{m_1 m_2}$, or over 660,000 numbers.

The computer program for the iterative solution differed in several minor respects from that described in Section III.3. In order to save machine time, the effective potential was computed for a rough mesh spacing, and the intermediate points were obtained by interpolation. Also, the extrapolation of the effective potential into the vacuum region was done by fitting an exponential of undetermined slope to the first two known points (rather than fitting an exponential of predetermined slope to one point).

Specifically, the program functioned in the following manner: During each iteration the computer begins with a table of $Q \left\{ \begin{smallmatrix} 0 \\ 1 \\ 11 \end{smallmatrix} \right\}_L(Z)$ for a Z -range of 10 fermis in intervals of $\frac{1}{3}$ fermi. It then performs the following calculations:

- 1) For a particular value of ω , a table of $V \left\{ \begin{smallmatrix} 0 \\ 1 \\ 11 \end{smallmatrix} \right\}(Z\omega)$ is computed

from the Q table by means of (5.15). The table of V is extended on each side by about 8 fermis. In the right-hand region, these functions are set

equal to their homogeneous-case values. On the left, they are extended by fitting an exponential $c_1 e^{-c_2 z}$ to the first two tabulated values.

2) The various derivatives and combinations of the V 's which appear in (3.45) are calculated, and these functions are interpolated to give a table with a spacing of $\frac{1}{12}$ fermi.

3) For given values of p_r and ω , a table of the wave function $\phi(z p_r \omega - (p_r^2/2m))$ is computed in the left-hand extension by assuming that the potential in (3.45) is an exponential.

4) The table of ϕ is computed for the main region of 10 fermis by point-to-point solution of (3.45), with the use of a modified Noumerov method with a mesh spacing of $\frac{1}{12}$ fermi.

5) The table of ϕ is extended into the right-hand region by fitting a sine function to the last two points in the main region, and these two points are also used to determine the normalization. The entire wave function is normalized according to (3.49), and (3.44) is used to obtain $\psi(z p_r \omega - (p_r^2/2m))$. This function is tabulated for a mesh spacing of $\frac{1}{6}$ fermi.

6) Steps 1) to 5) are repeated over various values of ω , with the number of values ranging from 4 to 28, depending upon the value of p_r .

7) The resulting table of wave functions is integrated over ω to obtain the functions $B_L(Z z p_r)$ defined by (5.18) for a spacing of $\frac{1}{6}$ fermi in Z and $\frac{1}{3}$ fermi in z .

8) The functions $C \left\{ \begin{smallmatrix} 0 \\ II \end{smallmatrix} \right\}_L(Z p_r)$ are obtained by summing the products of B and the Ψ -coefficients as in (5.26). In order to increase speed, this summation is truncated to exclude values of $\Psi_{m_1 m_2}$ smaller in magnitude than $10^{-4} \text{Max} |\Psi_{m_1 m_2}|$. The C 's are computed for a mesh spacing of $\frac{1}{3}$ fermi.

9) Steps 1) to 8) are repeated for 13 values of p_r , and a new table of $Q \left\{ \begin{smallmatrix} 0 \\ II \end{smallmatrix} \right\}_L(Z)$ is obtained by integrating the C 's as in (5.16). In a similar manner, (5.1) and (5.2) are used to obtain the density and energy density.

The computation was performed with the interparticle potential parameters in (4.101) and the homogeneous-case effective-mass results for the local-transport zero point.

After ten iterations, the result of each iteration was identical with the previous result, except for a slight displacement along the Z axis towards the vacuum side. This displacement was about $\frac{1}{75}$ fermi, which is small enough to be attributed to numerical errors in the spatial boundary conditions.

The resulting effective potential, after the tenth iteration, is shown in Figures 14 and 15, and tabulated in Appendix C. Figure 16 gives the

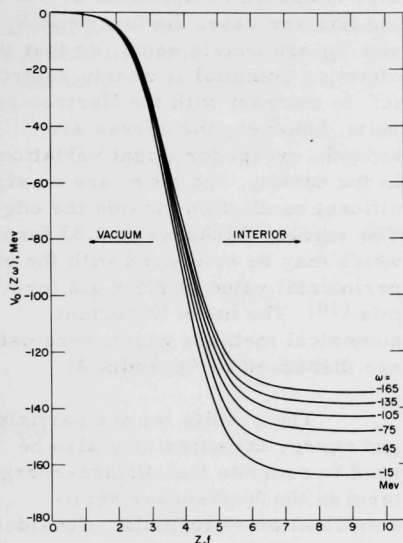
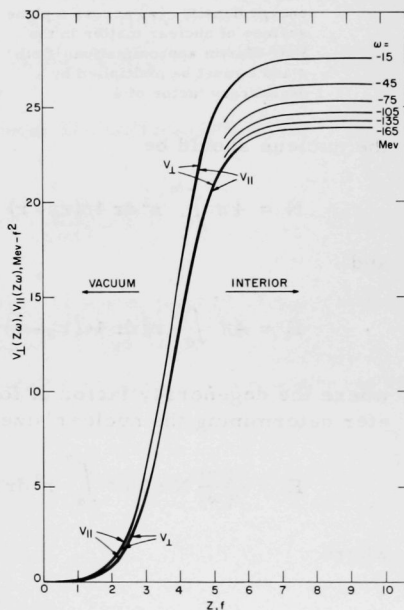


Fig. 14

The momentum-independent term $V_0(z, \omega)$ of the effective-mass approximation for the effective potential across a plane surface of nuclear matter in the Puff-Martin approximation. The quantity is given as a function of z for discrete ω . See footnote 5.

Fig. 15

The quadratic terms $V_I(z, \omega)$ and $V_{II}(z, \omega)$ of the effective-mass approximation for the effective potential across a plane surface of nuclear matter in the Puff-Martin approximation. These terms are given as functions of z for discrete ω . For clarity only the curves for $\omega = -15$ and -165 Mev are continued into the vacuum region. The two terms V_I and V_{II} , which are the components of the momentum perpendicular and parallel to the Z axis, are equal, to within the limited accuracy of the graph, except in the shoulder regions, where a small difference is indicated by splitting the curves. See footnote 5.



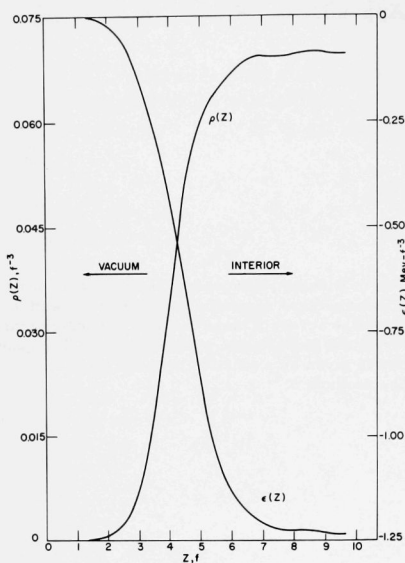


Fig. 16. The particle density $\rho(z)$ and the energy density $\epsilon(z)$ across a plane surface of nuclear matter in the Puff-Martin approximation. Both ρ and ϵ must be multiplied by a degeneracy factor of 4.

corresponding results for the particle and energy densities, which are also tabulated in Appendix C. As in the Hartree case, the functions V_{\perp} and V_{\parallel} are nearly equal, so that the effective potential is nearly isotropic. In contrast with the Hartree results, however, the curves are smooth, except for slight variations in the density, and there are no significant oscillations inside the edge. The surface thickness is 2.33 fermis, which may be compared with the experimental value of 2.5 ± 0.2 fermis.⁽¹⁰⁾ The more important numerical methods which were used are discussed in Appendix A.

The results for the particle and energy densities may also be used to compute the surface-energy term in the Weizsäcker semi-empirical mass formula. Consider a large spherical nucleus; its particle and energy densities, as functions of radial distance, should possess the same shape and height as our calculated $\rho(z)$ and $\epsilon(z)$. Thus, the total number of particles and energy of

the nucleus should be

$$N = 4\pi \int_0^{\infty} r^2 dr 4\rho(r_0 - r) \quad , \quad (5.27)$$

and

$$E = 4\pi \int_0^{\infty} r^2 dr 4\epsilon(r_0 - r) \quad , \quad (5.28)$$

where the degeneracy factor of four has been inserted, and r_0 is a parameter determining the nuclear size. Then

$$E = \frac{\epsilon(\infty)}{\rho(\infty)} N + 16\pi \int_0^{\infty} r^2 dr s(r_0 - r) \quad , \quad (5.29)$$

where

$$s(z) = \epsilon(z) - \frac{\epsilon(\infty)}{\rho(\infty)} \rho(z) \quad (5.30)$$

is a function which is nonzero only in a region near the surface. Thus, for a sufficiently large nucleus, the integration in equation (5.29) may be extended to negative r , and E may be rewritten as

$$\begin{aligned} E &= \frac{\epsilon(\infty)}{\rho(\infty)} N + 16\pi \int_{-\infty}^{\infty} (r_0 - z)^2 dz s(z) \\ &= \frac{\epsilon(\infty)}{\rho(\infty)} N + 16\pi r_0^2 \int_{-\infty}^{\infty} dz s(z) + 0(r_0) \quad . \end{aligned} \quad (5.31)$$

On the other hand,

$$N = \frac{16\pi}{3} \rho(\infty) r_0^3 + 0(r_0^2) \quad , \quad (5.32)$$

so that

$$\left[\frac{3N}{16\pi\rho(\infty)} \right]^{2/3} = r_0^2 + 0(r_0) \quad . \quad (5.33)$$

Thus

$$E = \frac{\epsilon(\infty)}{\rho(\infty)} N + 16\pi \left[\frac{3N}{16\pi\rho(\infty)} \right]^{2/3} \int_{-\infty}^{\infty} dz s(z) + 0(r_0) \quad . \quad (5.34)$$

A comparison with the Weizsäcker expansion $E = u_v N + u_s N^{2/3}$ determines the surface energy u_s to be

$$u_s = 16\pi \left[\frac{3}{16\pi\rho(\infty)} \right]^{2/3} \int_{-\infty}^{\infty} dz \left[\epsilon(z) - \frac{\epsilon(\infty)}{\rho(\infty)} \rho(z) \right] \quad . \quad (5.35)$$

A computation of the surface energy from the results of our calculation gives $u_s = 18.79$ Mev, which is in reasonable agreement with the empirical value of 17.804 Mev obtained by Green.⁽⁸⁾ Thus our calculation leads to reasonable values for both the surface thickness and surface energy.

APPENDIX A

NUMERICAL METHODS

A.1. Numerical Solution of the Schroedinger Equation

The one-dimensional Schroedinger equation may be written as

$$\phi^{(2)}(z) = g(z) \phi(z) \quad . \quad (A.1)$$

This equation may be solved numerically by expanding the second derivative in terms of the difference operators δ^n and using the resulting equations to determine $\phi(z)$ for a given z in terms of $\phi(z)$ for smaller z . Such a procedure gives a direct method of solution if the boundary conditions (exclusive of normalization) can be expressed at a single point.

Specifically, suppose that we have a table of $g(z)$ for a sequence of equally spaced points at intervals of length h . Given the initial conditions on $\phi(z)$ at z_0 , we wish to obtain a similar table of $\phi(z)$ for $z > z_0$. Let

$$\phi_n = \phi(z_0 + nh) \quad ; \quad g_n = g(z_0 + nh) \quad . \quad (A.2)$$

A Taylor series expansion of the second central difference of ϕ_n contains only even derivatives:

$$\begin{aligned} \delta^2 \phi_n &= \phi_{n+1} - 2\phi_n + \phi_{n-1} \\ &= h^2 \phi_n^{(2)} + \frac{1}{12} h^4 \phi_n^{(4)} + \frac{1}{360} h^6 \phi_n^{(6)} + \frac{1}{20160} h^8 \phi_n^{(8)} + \dots \end{aligned} \quad (A.3)$$

If we ignore all right-hand terms beyond the first, and substitute (A.1), we obtain an approximate equation, accurate to order h^2 , giving ϕ_{n+1} in terms of ϕ_n and ϕ_{n-1} :

$$\phi_{n+1} \cong 2\phi_n - \phi_{n-1} + h^2 g_n \phi_n \quad . \quad (A.4)$$

A better approximation, obtained by Noumerov's method, is accurate to order h^4 . Let

$$y_n = \phi_n - \frac{h^2}{12} \phi_n^{(2)} = \left[1 - \frac{h^2}{12} g_n \right] \phi_n \quad . \quad (A.5)$$

The function y_n has been chosen so that the expansion of $\delta^2 y_n$ does not contain an h^4 term. We have

$$\delta^2 y_n = \delta^2 \phi_n - \frac{h^2}{12} \delta^2 \phi_n^{(2)} = h^2 \phi_n^{(2)} - \frac{1}{240} h^6 \phi_n^{(6)} - \frac{11}{60480} h^8 \phi_n^{(8)} - \dots \quad (A.6)$$

By dropping the terms of order h^6 and higher, and substituting (A.1) and (A.5), we obtain Noumerov's approximation:

$$y_{n+1} \cong 2y_n - y_{n-1} + h^2 g_n \phi_n = 2y_n - y_{n-1} + \frac{h^2 g_n}{1 - \frac{h^2}{12} g_n} y_n \quad (\text{A.7})$$

The accuracy of this method can be improved further by including a correction which takes into account the h^6 term in (A.6). The procedure described here is a modification of a method developed by Rubenstein, Huse, and Machlup.⁽¹⁶⁾ The general form of the expansion (A.3),

$$\delta^2 = h^2 \frac{d^2}{dz^2} + \frac{1}{12} h^4 \frac{d^4}{dz^4} + \dots \quad (\text{A.8})$$

may be squared to obtain an expansion of δ^4 ;

$$\delta^4 = h^4 \frac{d^4}{dz^4} + \frac{h^6}{6} \frac{d^6}{dz^6} + \dots \quad (\text{A.9})$$

Now, let

$$u_n = \frac{h^2}{12} \phi_n^{(2)} = \frac{h^2}{12} g_n \phi_n = \frac{\frac{h^2}{12} g_n}{1 - \frac{h^2}{12} g_n} y_n \quad (\text{A.10})$$

By solving (A.9) for the operator $h^4 d^4/dz^4$ and applying the result to u_n , we obtain an expression for the sixth-order term in (A.6):

$$\frac{1}{240} h^6 \phi_n^{(6)} = \frac{1}{20} \delta^4 u_n - \frac{1}{1440} h^8 \phi_n^{(8)} - \dots \quad (\text{A.11})$$

Unfortunately, the fourth central difference of u_n contains u_{n+2} and cannot be evaluated directly. However, to order h^8 ,

$$\frac{1}{12} h^8 \phi_n^{(8)} = h^6 \frac{d^6}{dz^6} u_n \cong \delta^6 u_{n-1} = \delta^4 u_n - 2\delta^4 u_{n-1} + \delta^4 u_{n-2} \quad (\text{A.12})$$

This gives a usable approximation for $\delta^4 u_n$, which may be substituted into (A.11). When the result is substituted into (A.6), we obtain

$$\delta^2 y_n \cong 12u_n - \frac{1}{20} [2\delta^4 u_{n-1} - \delta^4 u_{n-2}] - \frac{221}{60480} h^8 \phi_n^{(8)} \quad (\text{A.13})$$

We drop the h^8 term, expand the central differences, and use (A.10) to express u_{n+1} in terms of y_{n+1} . This gives the approximation

$$\left[1 + \frac{1}{10} \frac{\frac{h^2}{12} g_{n+1}}{1 - \frac{h^2}{12} g_{n+1}} \right] y_{n+1} \approx 2y_n - y_{n-1} + 12 \frac{9}{20} u_n - \frac{4}{5} u_{n-1} + \frac{7}{10} u_{n-2} - \frac{3}{10} u_{n-3} + \frac{1}{20} u_{n-4} \quad , \quad (\text{A.14})$$

where the u_n are obtained from the y_n by (A.10).

In order to apply this method, the value of the wave function at five consecutive points must first be obtained from the initial conditions. In the inhomogeneous-case computations described in Chapters III and V, these values were obtained from an approximate analytic solution in the near-vacuum region.

A.2. Spatial Integration of the Wave Functions

In carrying out the Puff-Martin inhomogeneous-case computation of Chapter V, we must perform the double spatial integration (5.17) by means of an integration formula of the form (5.26), i.e., by a summation over a set of equally spaced points in Z and z . The essential problem is the derivation of such a formula for the subsidiary kernel function L defined by (5.21), i.e.,

$$I = \int dZ dz \, L_{\left\{ \begin{smallmatrix} 0 \\ \parallel \end{smallmatrix} \right\}}(Z \, z \, p_r) B_L(Z_0 + Z, z, p_{r2}) \\ \approx \sum_{m_1} \sum_{m_2} \Phi_{m_1 m_2 \left\{ \begin{smallmatrix} 0 \\ \parallel \end{smallmatrix} \right\}} L^{(p_r)} B_{\text{sym } L}(Z_0, m_1 h_1, m_2 h_2, p_{r2}) \quad , \quad (\text{A.15})$$

where

$$B_{\text{sym } L}(Z_0 \, Z \, z \, p_{r2}) = B_L(Z_0 + Z, z, p_{r2}) + B_L(Z_0 - Z, z, p_{r2}) \quad , \quad (\text{A.16})$$

since (5.19) and (5.20) give directly

$$\Psi_{m_1 m_2 \{i\} L}(p_{r2}) = \sum_j M_{ij} \frac{1}{\beta^3} e^{-\left(\frac{1}{\beta^2} + \frac{\alpha L}{m}\right) p_{r2}^2} \int_0^\infty p_r dp_r e^{-\left(\frac{1}{\beta^2} + \frac{\alpha L}{4m}\right) p_r^2} \\ \times \left\{ \begin{array}{ll} I_0(s) & ; \quad j = 0 \\ (p_{r2}^2 + p_r^2) I_0(s) - 2p_r p_{r2} I_1(s) & ; \quad j = \perp \\ I_0(s) & ; \quad j = \parallel \end{array} \right\} \Phi_{m_1 m_2 \{j\} L}(p_r) \Bigg|_{s = p_r p_{r2} \left(\frac{2}{\beta^2} + \frac{\alpha L}{m} \right)} \quad . \quad (\text{A.17})$$

The integration in (A.15) may be simplified by introducing the function

$$\bar{B} \left\{ \begin{smallmatrix} 0 \\ \parallel \end{smallmatrix} \right\}^L (Z_0 Z z p_{R2}) = \begin{cases} \sqrt{\frac{m}{\pi \alpha_L}} e^{-\frac{\eta_L}{\gamma_L^2} z^2} \int dz' \left\{ \frac{1}{\beta^2} - \frac{\beta^4}{4} \left(\frac{2}{\gamma_L} z - z' \right)^2 \right\} e^{-\sigma_L (z - z')^2} B_{\text{sym } L} (Z_0 Z z' p_{R2}) & (\text{if } \alpha_L \neq 0) \\ \left\{ \frac{1}{\beta^2} - \frac{\beta^4}{4} z^2 \right\} e^{-\frac{\beta^2 z^2}{4}} B_{\text{sym } L} (Z_0 Z z p_{R2}) & (\text{if } \alpha_L = 0), \end{cases} \quad (\text{A.18})$$

where

$$\eta_L = \left[\frac{4}{\beta^2} + \frac{\alpha_L}{m} \right]^{-1} ; \sigma_L = \frac{\beta^2}{4} + \frac{m}{\alpha_L} ; \gamma_L = 1 + \frac{\beta^2}{4\sigma_L} .$$

In terms of \bar{B} , the integration in (A.15) reduces to

$$I = \frac{6\beta\pi}{m} \sum_k C_{kL} \int dZ dz < \frac{p_R}{2}, Z+z \mid \tau_k \mid \frac{p_R}{2}, Z-z > \bar{B} \left\{ \begin{smallmatrix} 0 \\ \parallel \end{smallmatrix} \right\}^L (Z_0, Z, \gamma_L z, p_{R2}). \quad (\text{A.19})$$

Now, suppose that we know the values of $\bar{B}(Z_0 Z z p_{R2})$ at the same lattice points in Z and z at which we know the values of B , i.e., with a spacing of h_1 in Z and h_2 in z . To perform the integration in (A.19), we might approximate \bar{B} by means of Lagrangian interpolation in Z and z , using $2n+1$ points in each dimension:

$$f(Z) \cong \sum_{m=-n}^n L_m^n \left(\frac{Z}{h} - m_0 \right) f \left((m+m_0)h \right) \quad (\text{and similarly in } z), \quad (\text{A.20})$$

where

$$L_m^n(x) = \prod_{\substack{k=-n \\ k \neq m}}^n \frac{(x-k)}{(m-k)} . \quad (\text{A.21})$$

However, this approximation is only good when Z and z are in the interior of the rectangle formed by the $(2n+1)^2$ lattice points used in the interpolation. When Z (or z) is outside this rectangle, the interpolation becomes an extrapolation and the error increases as the $2n+1$ power of Z (or z). Unfortunately, the exponential decay of τ_{yy} and τ_{yc} in $Z \pm z$ is not sufficient to make the integral of this error negligible in the extrapolation region.

To circumvent this difficulty, we have used the device of varying the choice of interpolation points so that the central point of the interpolation rectangle is always the lattice point nearest to the point Z, z . This is equivalent to choosing m_0 in (A.20) to be the integer whose value is closest to Z/h . In this method, a large number of lattice points are involved in the approximate integration, but the allowable lattice spacing is unusually large.

Application of this approximation to \bar{B} gives

$$\bar{B}_{\left\{\begin{smallmatrix} 0 \\ \perp \\ \parallel \end{smallmatrix}\right\}L} (Z_0 z p_{r2}) \approx \sum_{m_1=-n}^n \sum_{m_2=-n}^n L_{m_1}^n \left(\frac{Z}{h_1} - r \left(\frac{Z}{h_1} \right) \right) L_{m_2}^n \left(\frac{z}{h_2} - r \left(\frac{z}{h_2} \right) \right) \\ \times \bar{B}_{\left\{\begin{smallmatrix} 0 \\ \perp \\ \parallel \end{smallmatrix}\right\}L} \left(Z_0, \left| \left(m_1 + r \left(\frac{Z}{h_1} \right) \right) h_1 \right|, \left| \left(m_2 + r \left(\frac{z}{h_2} \right) \right) h_2 \right|, p_{r2} \right), \quad (\text{A.22})$$

where $r(x)$ is the integer nearest to x . The absolute value of the arguments on the right-hand side have been introduced to take advantage of the symmetry of \bar{B} in Z and z . Substitution of (A.22) into (A.19) gives

$$I = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \phi_{m_1 m_2} L(p_r) \bar{B}_{\left\{\begin{smallmatrix} 0 \\ \perp \\ \parallel \end{smallmatrix}\right\}L} (Z_0, m_1 h_1, m_2 h_2, p_{r2}) \quad (\text{A.23})$$

where

$$\phi_{m_1 m_2} L(p_r) = \frac{6\beta\pi}{m} \sum_k C_{kL} \sum_{m_3=-n}^n \sum_{m_4=-n}^n \int dZ dz < \frac{p_r}{2}, Z+z \left| \tau_k \right| \frac{p_r}{2}, Z-z > \\ \times L_{m_3}^n \left(\frac{Z}{h_1} - r \left(\frac{Z}{h_1} \right) \right) L_{m_4}^n \left(\frac{\gamma_L z}{h_2} - r \left(\frac{\gamma_L z}{h_2} \right) \right) \delta \left| r \left(\frac{Z}{h_1} \right) + m_3 \right|, m_1 \left| r \left(\frac{\gamma_L z}{h_2} \right) + m_4 \right|, m_2 \quad (\text{A.24})$$

The choice of the mesh spacing and number of interpolation points may be determined by examining the maximum error of the interpolation formula (A.22). The computation described in Chapter V is made with the values $h_1 = \frac{1}{6}$ fermi, $h_2 = \frac{1}{3}$ fermi, and $n = 10$. An investigation of the error for these values gives an estimate of the relative error magnitude of 2×10^{-9} if \bar{B} is derived from wave functions with characteristic momenta less than $p = 2.5 \text{ f}^{-1}$. For $p = 3 \text{ f}^{-1}$, the relative error magnitude is about 10^{-7} .

We are still faced with the problem of integrating (A.24) numerically. At first sight, this task appears to be complicated by the discontinuities of the integrand. However, since (A.24) is only an intermediate step in the

integration of (A.19), it is sufficient to use any integration method which is accurate for evaluating (A.19), even though it may be highly inaccurate for (A.24) itself. On the other hand, knowledge of the integrand in (A.24) is not limited to the lattice points, so that Gaussian methods with unequally spaced points may be used. In practice, the integration was performed in the variables $Z_1 = Z + z$ and $Z_2 = Z - z$ by means of 8-point Gauss-Legendre quadrature and 25-point Gauss-Laguerre quadrature (depending on the particular form of τ_k). Furthermore, the integration points for which τ_k was less than 10^{-9} of its maximum were discarded. This restriction limits the non-zero values of $\phi_{m_1 m_2}$ to the region $m_1 = 0$ to 43 and $m_2 = 0$ to 34.

We must now express the values of \bar{B} at the lattice points in terms of the values of B_{sym} . Let g_{mL} be coefficients such that

$$\sqrt{\frac{m}{\pi \alpha_L}} \int dz e^{-\sigma_L z^2} f(z) \cong \sum_{m=-n_g}^{n_g} g_{mL} f(mh_2) \quad (A.25)$$

Then,

$$\left\{ \bar{B} \begin{Bmatrix} 0 \\ \perp \\ \parallel \end{Bmatrix} \right\}_L (Z_0, m_1 h_1, m_2 h_2, p_{r2}) \cong e^{-\frac{\eta_L}{\gamma_L^2} m_2^2 h_2^2} \times \sum_{m_3=-n_g}^{n_g} g_{m_3 L} \left\{ \frac{1}{\frac{\beta^2}{2} - \frac{\beta^4}{4} \left[\left(1 - \frac{2}{\gamma_L} \right) m_2 + m_3 \right]^2 h_2^2} \right\} B_{\text{sym } L} (Z_0, m_1 h_1, |m_2 + m_3| h_2, p_{r2}) \quad (A.26)$$

where the absolute value is again introduced to take advantage of the symmetry of B_{sym} . The substitution of (A.26) and (A.23) into (A.15) gives

$$\left\{ \phi_{m_1 m_2} \begin{Bmatrix} 0 \\ \perp \\ \parallel \end{Bmatrix} \right\}_L (p_r) = \sum_{m_4=0}^{34} \phi_{m_1 m_4 L} (p_r) e^{-\frac{\eta_L}{\gamma_L^2} m_4^2 h_2^2} \times \sum_{m_3=-n_g}^{n_g} g_{m_3 L} \left\{ \frac{1}{\frac{\beta^2}{2} - \frac{\beta^4}{4} \left[\left(1 - \frac{2}{\gamma_L} \right) m_4 + m_3 \right]^2 h_2^2} \right\} \delta_{|m_3 + m_4|, m_2} \quad (A.27)$$

If $n_g \leq 20$, then $\phi_{m_1 m_2}$ will be nonzero only in the region $m_1 = 0$ to 43, $m_2 = 0$ to 54, and the summation in (A.15) may be restricted to these values.

The choice of the coefficients g_{mL} depends upon the value of σ_L (and therefore α_L). For $\alpha_L = 0$, the value of σ_L is infinite and $g_{mL} = \delta_{m,0}$. On the other hand, for small σ we may use the simple approximation

$$\int_{-\infty}^{\infty} dz e^{-\sigma z^2} f(z) \cong h_2 \sum_{m=-\infty}^{\infty} f(mh_2) e^{-\sigma m^2 h_2^2} \quad (A.28)$$

E. T. Goodwin⁽¹⁷⁾ has shown that the error in this approximation decreases rapidly as $\sigma \rightarrow 0$, and an examination of the error term which he obtains shows that the relative error in using this method will have a magnitude of less than 10^{-9} when $\sigma \leq 2.75$. To limit the extent of the summation we discard the terms for which $g_{mL} < 10^{-9} g_{0L}$ (for all L). The worst case occurs for the smallest value $\sigma_L = 0.441$ and leads to $n_g = 20$.

In the intermediate range, in which $\sigma > 2.75$ but is still finite, we may approximate $f(z)$ by Lagrangian interpolation, using (A.20) with $m_0 = 0$. This gives

$$\int dz e^{-\sigma z^2} f(z) \cong \sum_{m=-n_g}^{n_g} f(mh_2) \int dz e^{-\sigma z^2} L_m^{n_g} \left(\frac{z}{h_2} \right) \quad (A.29)$$

Experimental trials with various test functions established that $n_g = 11$ is sufficient in this region.

The numerical calculation of the Ψ -coefficients was performed in two steps. First, a table of the 44×35 arrays $\phi_{m_1 m_2}$ was computed for 7 values of α_L and 12 values of p_r . Then, from this table a second table of the $44 \times 55 \times 3$ arrays $\Psi_{m_1 m_2} \left\{ \begin{smallmatrix} 0 \\ 1 \\ 11 \end{smallmatrix} \right\}$ was computed for 7 values of α_L and

13 values of p_{r2} . To evaluate the integral over p_r in (A.17), 12-point Gauss-Laguerre quadrature was used. The two computations required 7 and 3 hr of machine time, respectively.

In the Hartree-Fock computation described in Chapter III the integration of the product of the kernel and spectral functions reduces to a single integral of the spectral function times a Gaussian interparticle potential. In this calculation the approximation (A.28) was used.

A.3. Energy and Momentum Integrations

In the inhomogeneous-case computations for both the Hartree-Fock and the Puff-Martin approximations, the density, energy density, and effective potential are expressed as integrals of the spectral function (or the product of the spectral function and the kernel function) over the energy ω and the perpendicular momentum p_r , as in (5.1), (5.2), (5.16), and (5.18). In the Puff-Martin case, the integrals are complicated by the presence

of the exponential functions $e^{\alpha_L \omega}$. The choice of a numerical procedure for these integrations is quite critical, since the time required by the entire computation is proportional to the number of points ω, p_r at which the spectral function must be evaluated.

This choice is determined primarily by the strong exponential and sinusoidal behavior of the spectral function at the two extremes of the spatial interval over which the density and effective potential must be computed. This behavior may be roughly approximated by

$$A\left(Z, Z', p_r, \omega - \frac{p_r^2}{2m}\right) \sim \frac{1}{k} \begin{cases} k^2 e^{2KZ_0} & \text{left-hand region} \\ \sin^2 kZ_1 & \text{right-hand region,} \end{cases} \quad (\text{A.30})$$

where Z_0 (negative) and Z_1 (positive) are the approximate distances from the left and right end-points of the spatial interval to the edge of the nuclear surface, and

$$k = \left[\frac{\omega - V_{0\text{hom}}(\omega)}{V_{2\text{hom}}(\omega) + \frac{1}{2m}} - p_r^2 \right]^{\frac{1}{2}}; \quad K = [-2m\omega + p_r^2]^{\frac{1}{2}}. \quad (\text{A.31})$$

The energy integration may be expressed as

$$J(p_r) = \int_{h(p_r)}^{\mu} \frac{d\omega}{2\pi} e^{\alpha_L \omega} A\left(Z, Z', p_r, \omega - \frac{p_r^2}{2m}\right). \quad (\text{A.32})$$

We must approximate this integral by a weighted sum of the values of A for a finite set of values of ω . In addition, the choice of ω -values must be independent of α_L . Unfortunately, since the factor $e^{\alpha_L \omega}$ varies from a constant for $\alpha_L = 0$ to a strongly decaying function for $\alpha_L = 0.1$, a choice of ω -points which is optimum for one value of α_L will be poor for other values. The only reasonable procedure is to approximate kA by interpolation (obtaining the appropriate weights by integrating the interpolation coefficients) and to choose the ω -points to minimize the maximum interpolation error over the region of integration.

Thus, we are led to use Chebyshev interpolation. Specifically, let us interpolate $f = kA$ as a function of the variable $x(\omega)$ in the interval $x_0 = x(h(p_r))$ to $x_1 = x(\mu)$:

$$f(x) = \sum_{i=1}^n f\left(x_0 + \frac{x_1 - x_0}{2} (s_i + 1)\right) L_i^n \left(2 \frac{x - x_0}{x_1 - x_0} - 1\right) + E(x), \quad (\text{A.33})$$

where

$$s_i = -\cos \left[\frac{2i-1}{2n} \pi \right] \quad (\text{A.34})$$

and

$$L_i^n(s) = \prod_{\substack{j=1 \\ j \neq i}}^n \frac{s - s_j}{s_i - s_j} \quad (\text{A.35})$$

In the region $x_0 \leq x \leq x_1$ the interpolation error is

$$\left| E(x) \right| \leq \frac{2}{n!} \left[\frac{x_1 - x_0}{4} \right]^n \left| \frac{d^n f(\xi)}{dx^n} \right|, \quad (\text{A.36})$$

where $x_0 \leq \xi \leq x_1$.

Now, consider the behavior of the n th-order derivative for the two test functions in (A.30). If $x(\omega)$ is slowly varying compared with the factors e^{2kZ_0} and $\sin^2 kZ_1$, then the dominant term in the derivative will be

$$\left| \frac{d^n f}{dx^n} \right| \sim \begin{cases} \left| \left(2Z_0 \frac{dK}{dx} \right)^n f \right| & \text{left-hand region} \\ \left| \left(2Z_1 \frac{dk}{dx} \right)^n f \right| & \text{right-hand region} \end{cases} \quad (\text{A.37})$$

The maximum of the error expression (A.36) will involve the maximum of (A.37), so that we wish to minimize the variation of (A.37) over the integration region. If we were concerned with only one of the two cases in (A.37), we would choose $x = K$ or $x = k$. To deal with both cases, it is necessary to make some compromise between these extremes such that $\left| 2Z_0 \frac{dK}{dx} \right|$ and $\left| 2Z_1 \frac{dk}{dx} \right|$ are both bounded, but neither quantity falls unnecessarily far below the bound. A reasonable choice is that $x(\omega)$ satisfy

$$dx^2 = (2Z_1 dk)^2 + (2Z_0 dK)^2 \quad (\text{A.38})$$

In the region of integration the function $K(k)$ is closely approximated by

$$K \cong [6.66 - 0.92 p_T^2 - 1.92 k^2]^{\frac{1}{2}} \quad (\text{A.39})$$

In general, (A.38) and (A.39) determine x to be an elliptic function of k . However, if we choose the special case $|Z_1| = \sqrt{1.92} |Z_0|$, the elliptic function reduces to a spherical function:

$$x = 2 |Z_0| K_0 \arcsin \frac{\sqrt{1.92} k}{K_0} \quad , \quad (\text{A.40})$$

where

$$K_0 = K(k=0) = \sqrt{-2mV_{\text{hom}}(p_r)} \quad . \quad (\text{A.41})$$

The choice of $|Z_1| = \sqrt{1.92} |Z_0|$ is essentially a weighting of the two test cases in determining the optimum integration method, and it is usable since Z_0 and Z_1 are roughly estimated quantities of about the same magnitude.

The variable k ranges from 0 to $\sqrt{p_f^2 - p_r^2}$ over the range of integration in (A.32). Therefore, (18)

$$x_0 = 0 \quad ; \quad x_1 = 2 |Z_0| K_0 \arcsin \frac{\sqrt{1.92} \sqrt{p_f^2 - p_r^2}}{K_0} \quad . \quad (\text{A.42})$$

If we substitute (A.40) and (A.42) into the interpolation approximation (A.33) for kA and substitute the result into (A.32), we obtain

$$J(p_r) \cong \sum_{i=1}^n H_i^{(\omega)}(\alpha_L p_r) A \left(Z Z' p_r \omega_i - \frac{p_r^2}{2m} \right) \quad , \quad (\text{A.43})$$

where

$$\omega_i = \omega(x_i) \quad ; \quad x_i = \frac{x_1}{2} (s_i + 1) \quad , \quad (\text{A.44})$$

and

$$H_i^{(\omega)}(\alpha_L p_r) = k(\omega_i) \int_{h(p_r)}^{\mu} \frac{d\omega}{2\pi} e^{\alpha_L \omega} \frac{1}{k(\omega)} L_i^n \left(\frac{2x(\omega)}{x_1} - 1 \right) \quad . \quad (\text{A.45})$$

The integration over the perpendicular momentum p_r is simply

$$I = \int_0^{p_f} \frac{p_r dp_r}{2\pi} J(p_r) \quad . \quad (\text{A.46})$$

(In forming the effective potential the integrand also involves the kernel K , but this is slowly varying in p_r as compared with J and may be ignored in determining the integration method.) This integral may be treated in a

manner similar to the energy integral. To obtain test functions, the integral (A.32) of each of the functions in (A.30) may be roughly approximated by a linear combination of two terms with exponential (or sinusoidal) behavior corresponding to the values of K (or k) at the end points of the energy integration, $\omega = h(p_r)$ and $\omega = \mu$. This leads to four test functions, one of which [corresponding to $k = 0$ when $\omega = h(p_r)$] is a trivial constant. The remaining three are

$$J(p_r) \sim \begin{cases} e^{2K_0 Z_0} & \text{left-hand region, } \omega = h(p_r) \\ e^{2K_1 Z_0} & \text{left-hand region, } \omega = \mu \\ \sin 2kZ_1 & \text{right-hand region, } \omega = \mu \end{cases}, \quad (\text{A.47})$$

where

$$K_0 = \sqrt{-2mV_{\text{hom}}(p_r)} \quad ; \quad K_1 = \sqrt{-2m\mu + p_r^2} \quad ; \quad k = \sqrt{p_f^2 - p_r^2} \quad . \quad (\text{A.48})$$

Let us integrate J as a function of the variable $q = q(p_r)$. In the same manner as before, q should be chosen so that $\left| 2Z_0 \frac{dK_0}{dq} \right|$, $\left| 2Z_0 \frac{dK_1}{dq} \right|$, and $\left| 2Z_1 \frac{dk}{dq} \right|$ are all bounded, and kept as close to the bound as possible. If we substitute (A.39) into (A.48), we find that $|dK_0| \leq 0.92 |dK_1|$, so that the K_0 case may be ignored and q chosen as a compromise between $q = K_1$ and $q = k$. As before, we choose

$$dq^2 = (2Z_0 dK_1)^2 + (2Z_1 dk)^2 \quad (\text{A.49})$$

With the substitution of (A.48) and (A.39), we obtain an elliptic function which degenerates into a circular function for $|Z_1| = |Z_0|$. In this case,

$$q = 2 |Z_1| K_{00} \arcsin \frac{k}{K_{00}} \quad , \quad (\text{A.50})$$

where

$$K_{00} = \sqrt{-2m\mu + p_f^2} \quad . \quad (\text{A.51})$$

As p_r goes from p_f to zero, $k = \sqrt{p_f^2 - p_r^2}$ goes from zero to p_f , and q goes from

$$q_0 = 0 \quad \text{to} \quad q_1 = 2 |Z_1| K_{00} \arcsin \frac{p_f}{K_{00}} \quad . \quad (\text{A.52})$$

In carrying out the integration over q , we are no longer faced with a wide variety of integrals for different α_L . As a result, we may optimize the integration error itself, rather than the interpolation error, by using Gauss-Legendre quadrature. The resulting approximation is

$$I \approx \frac{q_1}{8\pi |Z_1|} \sum_{j=1}^n H_j k_j \left[1 - \frac{k_j^2}{K_{00}^2} \right]^{\frac{1}{2}} J \left(\sqrt{p_f^2 - k_j^2} \right), \quad (\text{A.53})$$

where

$$k_j = K_{00} \sin \left[\frac{q_1}{2 |Z_0| K_{00}} \frac{(x_j + 1)}{2} \right], \quad (\text{A.54})$$

and x_j and H_j are the abscissas and weights for Gauss-Legendre quadrature over the interval -1 to $+1$.

In the Puff-Martin computation these methods were used with 13 points for the p_r -integration and 4 to 28 points (depending on the integration range) for the ω -integration. The accuracy was tested by applying the method (with a varying number of points) to the trial function (A.30) and to the computation of the density $\rho(Z)$ from the initial estimate for the effective potential. The largest relative errors were about 10^{-5} .

This method was not used for the Hartree-Fock calculation. In that case, Gauss-Legendre quadrature was used in the variables $\sqrt{\omega - V_0 - V_2 p_r^2}$ and $\sqrt{p_f^2 - p_r^2}$.

A.4. Methods for the Homogeneous Puff-Martin Computation

In performing the homogeneous-case computation for the Puff-Martin approximation, it is necessary to obtain the solutions $V(p)$ and $\rho(p)$ of the simultaneous equations (4.86) and (4.87). This is done by iteration of a multidimensional Newton-Raphson procedure.

Let x_k and H_k be abscissas and weights for n -point Gauss-Legendre quadrature over the interval from -1 to $+1$. (Ten points were used in the computation described in Chapter IV.) Then the momentum integrations in (4.86) and (4.87) may be approximated by

$$\int_{|p| < p_f} (dp) f(p) = 4\pi \int_0^{p_f} p^2 dp f(p) \approx \sum_{k=1}^n \bar{H}_k f(p_k), \quad (\text{A.55})$$

where

$$p_k = \frac{p_f}{2} (x_k + 1) \quad ; \quad \bar{H}_k = 2\pi p_f H_k p_k^2. \quad (\text{A.56})$$

Using this approximation, (4.86) and (4.87) may be written as a set of $2n$ equations for the $2n$ values of V and ρ at the integration points:

$$F_k = V_k - \sum_{j=1}^n \bar{H}_j K \left(p_k, p_j, \frac{p_k^2 + p_j^2}{2m} + V_k + V_j \right) \rho_j = 0 \quad (\text{A.57})$$

and

$$G_k = \rho_k \left[1 - \sum_{j=1}^n \bar{H}_j \frac{\partial}{\partial \omega} K \left(p_k, p_j, \frac{p_k^2 + p_j^2}{2m} + V_k + V_j \right) \rho_j \right] - 1 = 0 \quad , \quad (\text{A.58})$$

where

$$V_k = V(p_k) \quad ; \quad \rho_k = \rho(p_k) \quad . \quad (\text{A.59})$$

The independent variables V_k , ρ_k may be considered as a $2n$ -dimensional vector:

$$\vec{v} = [V_1 \dots V_n \rho_1 \dots \rho_n] \quad . \quad (\text{A.60})$$

Similarly, the dependent variables F_k , G_k may be combined into

$$\vec{F} = [F_1 \dots F_n G_1 \dots G_n] \quad . \quad (\text{A.61})$$

In this formalism, (A.57) and (A.58) become the vector equation

$$\vec{F}(\vec{v}) = 0 \quad . \quad (\text{A.62})$$

Now let \vec{v}_n be a trial solution of (A.62). To find a better solution \vec{v}_{n+1} , we expand \vec{F} in (A.62) in a Taylor series about \vec{v}_n , retaining the first two terms. The solution \vec{v}_{n+1} is taken to be the solution of the resulting approximate equation:

$$\vec{F}(\vec{v}_n) + \frac{\partial \vec{F}(\vec{v}_n)}{\partial \vec{v}} \cdot [\vec{v}_{n+1} - \vec{v}_n] = 0 \quad . \quad (\text{A.63})$$

This is a $2n$ -dimensional linear equation involving the $2n$ -by- $2n$ matrix $\partial \vec{F} / \partial \vec{v}$. By inverting this matrix, we obtain

$$\vec{v}_{n+1} = \vec{v}_n - \left[\frac{\partial \vec{F}(\vec{v}_n)}{\partial \vec{v}} \right]^{-1} \cdot \vec{F}(\vec{v}_n) \quad . \quad (\text{A.64})$$

The iteration of (A.64) produces the desired values of V and ρ . Since the error of the Taylor approximation decreases as the square of the difference $\vec{v}_{n+1} - \vec{v}_n$, the convergence is very rapid. The derivative of \vec{F} is given by differentiation of (A.57) and (A.58), and involves the function K and its first two derivatives with respect to energy.

This method yields a solution of (4.86) and (4.87) for a particular value of p_f . In the computations of Section IV.3, the method is iterated to obtain a solution for a particular zero point. This is done in the following manner: When V and ρ have been obtained for a given p_f , they are used to compute the pressure $P(p_f)$ (using whichever pressure expression is of interest). After this function has been computed at two points, $P_n = P(p_{fn})$ and $P_{n-1} = P(p_{fn-1})$, it may be approximated by a linear function passing through these points:

$$P(p_f) \cong \frac{P_n p_{fn} - P_{n-1} p_{fn-1} + (P_n - P_{n-1}) p_f}{p_{fn} - p_{fn-1}} \quad . \quad (A.65)$$

A new value of p_f is then obtained by solving $P(p_f) = 0$ in this linear approximation;

$$p_{fn+1} = (P_n p_{fn-1} - P_{n-1} p_{fn}) (P_n - P_{n-1})^{-1} \quad , \quad (A.66)$$

and then evaluating the pressure at the new p_f . The repetition of this procedure converges upon a value of p_f for which $P(p_f) = 0$. At each stage the two points used in (A.66) are chosen to be the last point computed and one of the two points used in the previous stage (whichever one is nearer to the last point computed).

APPENDIX B

ADDITIONAL RESULTS OF THE HOMOGENEOUS-CASE
PUFF-MARTIN COMPUTATION

The following tables give additional results from the computations described in Chapter IV. Each table gives the functions $V(p)$ and $\rho(p)$ for a particular value of p_f , along with the parameters μ , ρ , ϵ , P_μ , and P_{L-T} . The first eight tables give these results for equally spaced values of $p_f = 0.6(0.2)2.0$, the next two tables give results for the μ and L-T zero points, and the last table gives results for the L-T zero point using the effective-mass approximation. The appropriate units are

p_f	fermi ⁻¹	ρ	fermi ⁻³
p	fermi ⁻¹	ϵ	Mev-f ⁻³
$V(p)$	Mev	P_μ	Mev-f ⁻³
μ	Mev	P_{L-T}	Mev-f ⁻³
β fermi ⁻¹			

The tables have been reproduced directly from a listing of the computer output (except for the μ -zero-point table). The least significant figures are unrounded in some cases.

Note that the quantities ρ , ϵ , P_μ , and P_{L-T} must be multiplied by a degeneracy factor of four.

EXACT SOLUTION

PF = 0.60000
 MU = -6.9359
 RHO = 0.002967
 EPSILON = -0.00825
 MU PRESSURE = -0.01232
 L-T PRESSURE = -0.01032

P/PF	P	V(P)	RHO(P)
0.98695	0.59217	-14.403	0.79647
0.93253	0.55952	-14.415	0.80174
0.83970	0.50382	-14.440	0.80946
0.71670	0.43002	-14.478	0.81764
0.57444	0.34466	-14.523	0.82480
0.42556	0.25534	-14.564	0.83015
0.28330	0.16998	-14.595	0.83358
0.16030	0.09618	-14.613	0.83537
0.06747	0.04048	-14.620	0.83605
0.01305	0.00783	-14.621	0.83619

EXACT SOLUTION

PF = 0.80000
 MU = -12.9995
 RHO = 0.007406
 EPSILON = -0.04191
 MU PRESSURE = -0.05436
 L-T PRESSURE = -0.04690

P/PF	P	V(P)	RHO(P)
0.98695	0.78956	-26.325	0.84548
0.93253	0.74603	-26.550	0.84898
0.83970	0.67176	-26.918	0.85408
0.71670	0.57336	-27.365	0.85943
0.57444	0.45955	-27.813	0.86407
0.42556	0.34045	-28.189	0.86751
0.28330	0.22664	-28.450	0.86971
0.16030	0.12824	-28.593	0.87085
0.06747	0.05397	-28.649	0.87128
0.01305	0.01044	-28.661	0.87137

EXACT SOLUTION

PF = 1.00000
 MU = -20.1648
 RHO = 0.014830
 EPSILON = -0.14038
 MU PRESSURE = -0.15865
 L-T PRESSURE = -0.13638

P/PF	P	V(P)	RHO(P)
0.98695	0.98695	-41.073	0.87020
0.93253	0.93253	-41.781	0.87276
0.83970	0.83970	-42.930	0.87645
0.71670	0.71670	-44.321	0.88026
0.57444	0.57444	-45.709	0.88353
0.42556	0.42556	-46.873	0.88592
0.28330	0.28330	-47.682	0.88744
0.16030	0.16030	-48.126	0.88822
0.06747	0.06747	-48.300	0.88852
0.01305	0.01305	-48.336	0.88858

EXACT SOLUTION

PF = 1.20000
 MU = -26.4912
 RHO = 0.025842
 EPSILON = -0.34750
 MU PRESSURE = -0.33709
 L-T PRESSURE = -0.27767

P/PF	P	V(P)	RHO(P)
0.98695	1.18434	-56.728	0.87920
0.93253	1.11904	-58.282	0.88129
0.83970	1.00765	-60.816	0.88427
0.71670	0.86004	-63.902	0.88729
0.57444	0.68932	-67.006	0.88984
0.42556	0.51068	-69.628	0.89169
0.28330	0.33996	-71.459	0.89285
0.16030	0.19235	-72.468	0.89345
0.06747	0.08096	-72.863	0.89367
0.01305	0.01566	-72.945	0.89372

EXACT SOLUTION

PF = 1.40000
 MU = -29.5632
 RHO = 0.040885
 EPSILON = -0.67488
 MU PRESSURE = -0.53381
 L-T PRESSURE = -0.38593

P/PF	P	V(P)	RHO(P)
0.98695	1.38173	-70.883	0.87633
0.93253	1.30554	-73.680	0.87834
0.83970	1.17559	-78.277	0.88114
0.71670	1.00338	-83.932	0.88394
0.57444	0.80421	-89.682	0.88625
0.42556	0.59579	-94.586	0.88792
0.28330	0.39662	-98.036	0.88895
0.16030	0.22441	-99.948	0.88948
0.06747	0.09446	-100.697	0.88968
0.01305	0.01827	-100.853	0.88972

EXACT SOLUTION

PF = 1.60000
 MU = -27.1606
 RHO = 0.060211
 EPSILON = -1.05317
 MU PRESSURE = -0.58220
 L-T PRESSURE = -0.23624

P/PF	P	V(P)	RHO(P)
0.98695	1.57913	-81.303	0.86370
0.93253	1.49205	-85.690	0.86605
0.83970	1.34353	-92.969	0.86923
0.71670	1.14672	-102.034	0.87233
0.57444	0.91910	-111.365	0.87487
0.42556	0.68090	-119.408	0.87667
0.28330	0.45328	-125.113	0.87778
0.16030	0.25647	-128.289	0.87835
0.06747	0.10795	-129.536	0.87857
0.01305	0.02087	-129.796	0.87861

EXACT SOLUTION

PF = 1.80000
 MU = -17.8419
 RHO = 0.083850
 EPSILON = -1.29668
 MU PRESSURE = -0.19935
 L-T PRESSURE = 0.55739

P/PF	P	V(P)	RHO(P)
0.98695	1.77652	-86.510	0.84208
0.93253	1.67856	-92.695	0.84548
0.83970	1.51147	-103.071	0.84984
0.71670	1.29006	-116.170	0.85393
0.57444	1.03399	-129.836	0.85720
0.42556	0.76601	-141.751	0.85949
0.28330	0.50994	-150.271	0.86090
0.16030	0.28853	-155.038	0.86162
0.06747	0.12144	-156.915	0.86189
0.01305	0.02348	-157.306	0.86194

EXACT SOLUTION

PF = 2.00000
 MU = -1.3085
 RHO = 0.111501
 EPSILON = -1.10553
 MU PRESSURE = 0.95963
 L-T PRESSURE = 2.49883

P/PF	P	V(P)	RHO(P)
0.98695	1.97391	-86.133	0.80842
0.93253	1.86506	-94.076	0.81623
0.83970	1.67941	-107.617	0.82358
0.71670	1.43340	-124.993	0.82975
0.57444	1.14887	-143.391	0.83444
0.42556	0.85113	-159.625	0.83766
0.28330	0.56660	-171.330	0.83961
0.16030	0.32059	-177.912	0.84060
0.06747	0.13494	-180.510	0.84097
0.01305	0.02609	-181.051	0.84105

EXACT SOLUTION

PF = 1.8491
 MU = -14.447
 RHO = 0.09028
 EPSILON = -1.3034
 MU PRESSURE = 0.0000
 L-T PRESSURE = 0.9073

P/PF	P	V(P)	RHO(P)
0.98695	1.8249	-86.92	0.8353
0.93253	1.7243	-93.55	0.8392
0.83970	1.5527	-104.72	0.8440
0.71670	1.3252	-118.86	0.8485
0.57444	1.0622	-133.67	0.8520
0.42556	0.7869	-146.62	0.8545
0.28330	0.5238	-155.89	0.8560
0.16030	0.2964	-161.09	0.8568
0.06747	0.1248	-163.14	0.8571
0.01305	0.0241	-163.56	0.8572

EXACT SOLUTION

PF = 1.68645
 MU = -24.0275
 RHO = 0.069908
 EPSILON = -1.19026
 MU PRESSURE = -0.48945
 L-T PRESSURE = -0.00000

P/PF	P	V(P)	RHO(P)
0.98695	1.66445	-84.243	0.85547
0.93253	1.57267	-89.393	0.85815
0.83970	1.41612	-97.977	0.86171
0.71670	1.20868	-108.728	0.86515
0.57444	0.96876	-119.857	0.86793
0.42556	0.71769	-129.498	0.86989
0.28330	0.47778	-136.359	0.87111
0.16030	0.27033	-140.187	0.87173
0.06747	0.11378	-141.693	0.87196
0.01305	0.02200	-142.006	0.87201

EFFECTIVE MASS SOLUTION WITH BETA = 0.89307

PF = 1.68645
 MU = -24.7664
 RHO = 0.069823
 EPSILON = -1.23233
 MU PRESSURE = -0.49694
 L-T PRESSURE = -0.00000

P/PF	P	V(P)	RHO(P)
0.98695	1.66445	-85.218	0.85522
0.93253	1.57267	-91.105	0.85636
0.83970	1.41612	-100.193	0.85946
0.71670	1.20868	-110.591	0.86372
0.57444	0.96876	-120.454	0.86780
0.42556	0.71769	-128.394	0.87092
0.28330	0.47778	-133.752	0.87292
0.16030	0.27033	-136.645	0.87396
0.06747	0.11378	-137.766	0.87436
0.01305	0.02200	-137.998	0.87444

APPENDIX C

ADDITIONAL RESULTS OF THE INHOMOGENEOUS-CASE
PUFF-MARTIN COMPUTATION

The following tables give additional results from the computation described in Chapter V, after the tenth iteration. The tabulated functions are the density $\rho(z)$, the energy density $\epsilon(z)$, and the three components $V_0(z\omega)$, $V_{\perp}(z\omega)$, and $V_{\parallel}(z\omega)$ of the effective potential.⁽⁵⁾ The appropriate units are

z	fermi	ϵ	Mev-f ⁻³
ω	Mev	V_0	Mev
ρ	fermi ⁻³	V_{\perp}, \parallel	Mev-f ²

The tables have been reproduced directly from a listing of the computer output. The least significant figures are unrounded in some cases.

Note that the functions $\rho(z)$ and $\epsilon(z)$ must be multiplied by a degeneracy factor of 4.

DENSITY

ENERGY DENSITY

EFFECTIVE POTENTIAL FOR OMEGA = -165.00 MEV

Z	RHO	Z	EPSILON	Z	V ZERO	V PERP	V PARL
0.	0.00000	0.	-0.00008	0.	-0.04	0.01	0.01
0.33	0.00001	0.33	-0.00021	0.33	-0.09	0.01	0.02
0.67	0.00002	0.67	-0.00052	0.67	-0.22	0.03	0.04
1.00	0.00004	1.00	-0.00131	1.00	-0.51	0.07	0.09
1.33	0.00010	1.33	-0.00331	1.33	-1.18	0.17	0.21
1.67	0.00025	1.67	-0.00826	1.67	-2.59	0.37	0.43
2.00	0.00064	2.00	-0.01982	2.00	-5.37	0.76	0.86
2.33	0.00156	2.33	-0.04414	2.33	-10.38	1.50	1.63
2.67	0.00360	2.67	-0.08781	2.67	-18.41	2.74	2.88
3.00	0.00762	3.00	-0.15222	3.00	-29.81	4.63	4.75
3.33	0.01443	3.33	-0.23215	3.33	-44.11	7.21	7.26
3.67	0.02403	3.67	-0.32531	3.67	-60.11	10.31	10.28
4.00	0.03522	4.00	-0.43765	4.00	-76.32	13.61	13.48
4.33	0.04600	4.33	-0.57278	4.33	-91.36	16.67	16.48
4.67	0.05452	4.67	-0.72227	4.67	-104.21	19.14	18.95
5.00	0.06006	5.00	-0.86840	5.00	-114.31	20.88	20.74
5.33	0.06320	5.33	-0.99182	5.33	-121.59	22.00	21.91
5.67	0.06512	5.67	-1.07942	5.67	-126.36	22.68	22.65
6.00	0.06672	6.00	-1.13182	6.00	-129.23	23.14	23.13
6.33	0.06813	6.33	-1.16223	6.33	-130.94	23.46	23.46
6.67	0.06902	6.67	-1.18450	6.67	-132.08	23.67	23.67
7.00	0.06929	7.00	-1.20383	7.00	-132.95	23.78	23.78
7.33	0.06923	7.33	-1.21808	7.33	-133.55	23.83	23.83
7.67	0.06926	7.67	-1.22452	7.67	-133.87	23.86	23.86
8.00	0.06952	8.00	-1.22499	8.00	-133.97	23.90	23.90
8.33	0.06982	8.33	-1.22460	8.33	-134.01	23.94	23.93
8.67	0.06991	8.67	-1.22691	8.67	-134.09	23.95	23.95
9.00	0.06977	9.00	-1.23045	9.00	-134.23	23.95	23.95
9.33	0.06962	9.33	-1.23390	9.33	-134.32	23.94	23.94
9.67	0.06965	9.67	-1.23157	9.67	-134.33	23.94	23.94

EFFECTIVE POTENTIAL FOR OMEGA = -150.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.09	0.01	0.02
0.67	-0.22	0.03	0.04
1.00	-0.52	0.07	0.10
1.33	-1.19	0.17	0.21
1.67	-2.62	0.37	0.44
2.00	-5.43	0.77	0.87
2.33	-10.49	1.51	1.64
2.67	-18.62	2.77	2.90
3.00	-30.17	4.68	4.79
3.33	-44.69	7.27	7.32
3.67	-60.96	10.40	10.36
4.00	-77.47	13.72	13.59
4.33	-92.79	16.79	16.62
4.67	-105.84	19.28	19.10
5.00	-116.08	21.03	20.89
5.33	-123.44	22.15	22.07
5.67	-128.26	22.84	22.81
6.00	-131.17	23.30	23.29
6.33	-132.90	23.62	23.62
6.67	-134.07	23.83	23.83
7.00	-134.94	23.94	23.94
7.33	-135.54	23.99	23.99
7.67	-135.86	24.02	24.02
8.00	-135.96	24.06	24.06
8.33	-136.01	24.10	24.09
8.67	-136.10	24.11	24.11
9.00	-136.22	24.11	24.11
9.33	-136.31	24.10	24.10
9.67	-136.32	24.10	24.10

EFFECTIVE POTENTIAL FOR OMEGA = -135.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.09	0.01	0.02
0.67	-0.22	0.03	0.04
1.00	-0.52	0.08	0.10
1.33	-1.20	0.17	0.21
1.67	-2.65	0.38	0.44
2.00	-5.50	0.78	0.88
2.33	-10.62	1.53	1.65
2.67	-18.85	2.80	2.93
3.00	-30.57	4.73	4.83
3.33	-45.31	7.35	7.39
3.67	-61.87	10.50	10.46
4.00	-78.69	13.84	13.72
4.33	-94.30	16.94	16.77
4.67	-107.58	19.44	19.27
5.00	-117.96	21.20	21.07
5.33	-125.40	22.33	22.25
5.67	-130.26	23.02	22.98
6.00	-133.21	23.48	23.47
6.33	-134.97	23.80	23.80
6.67	-136.15	24.01	24.01
7.00	-137.03	24.12	24.12
7.33	-137.64	24.17	24.17
7.67	-137.95	24.20	24.20
8.00	-138.06	24.24	24.24
8.33	-138.11	24.28	24.28
8.67	-138.20	24.29	24.29
9.00	-138.33	24.29	24.29
9.33	-138.41	24.28	24.28
9.67	-138.42	24.28	24.28

EFFECTIVE POTENTIAL FOR OMEGA = -120.00 MEV

	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.09	0.01	0.02
0.67	-0.23	0.03	0.04
1.00	-0.53	0.08	0.10
1.33	-1.22	0.17	0.21
1.67	-2.68	0.38	0.44
2.00	-5.57	0.79	0.89
2.33	-10.76	1.56	1.67
2.67	-19.11	2.84	2.96
3.00	-31.00	4.79	4.88
3.33	-45.99	7.44	7.47
3.67	-62.86	10.62	10.58
4.00	-80.01	13.99	13.87
4.33	-95.92	17.11	16.95
4.67	-109.43	19.63	19.47
5.00	-119.96	21.40	21.28
5.33	-127.48	22.53	22.45
5.67	-132.39	23.22	23.19
6.00	-135.37	23.68	23.67
6.33	-137.17	24.01	24.01
6.67	-138.37	24.22	24.22
7.00	-139.25	24.33	24.33
7.33	-139.85	24.37	24.38
7.67	-140.17	24.40	24.41
8.00	-140.28	24.44	24.44
8.33	-140.34	24.48	24.48
8.67	-140.43	24.50	24.50
9.00	-140.56	24.50	24.50
9.33	-140.64	24.49	24.49
9.67	-140.65	24.49	24.49

EFFECTIVE POTENTIAL FOR OMEGA = -105.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.09	0.01	0.02
0.67	-0.23	0.03	0.04
1.00	-0.54	0.08	0.10
1.33	-1.24	0.18	0.22
1.67	-2.73	0.39	0.45
2.00	-5.65	0.81	0.90
2.33	-10.92	1.58	1.69
2.67	-19.40	2.88	3.00
3.00	-31.49	4.86	4.95
3.33	-46.75	7.54	7.57
3.67	-63.95	10.76	10.71
4.00	-81.45	14.16	14.05
4.33	-97.68	17.31	17.16
4.67	-111.44	19.84	19.69
5.00	-122.12	21.63	21.51
5.33	-129.72	22.76	22.69
5.67	-134.68	23.46	23.42
6.00	-137.70	23.92	23.91
6.33	-139.52	24.24	24.24
6.67	-140.74	24.46	24.46
7.00	-141.63	24.57	24.57
7.33	-142.23	24.61	24.61
7.67	-142.55	24.64	24.64
8.00	-142.66	24.68	24.68
8.33	-142.73	24.72	24.72
8.67	-142.82	24.74	24.74
9.00	-142.94	24.73	24.73
9.33	-143.02	24.72	24.72
9.67	-143.03	24.73	24.73

EFFECTIVE POTENTIAL FOR OMEGA = -90.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.10	0.01	0.02
0.67	-0.23	0.03	0.04
1.00	-0.55	0.08	0.10
1.33	-1.26	0.18	0.22
1.67	-2.77	0.40	0.46
2.00	-5.75	0.83	0.91
2.33	-11.11	1.61	1.72
2.67	-19.73	2.94	3.04
3.00	-32.04	4.94	5.02
3.33	-47.60	7.66	7.68
3.67	-65.16	10.92	10.87
4.00	-83.05	14.36	14.25
4.33	-99.62	17.54	17.40
4.67	-113.63	20.10	19.96
5.00	-124.47	21.90	21.79
5.33	-132.16	23.04	22.97
5.67	-137.17	23.74	23.70
6.00	-140.21	24.20	24.19
6.33	-142.07	24.52	24.52
6.67	-143.30	24.73	24.74
7.00	-144.20	24.84	24.85
7.33	-144.80	24.89	24.89
7.67	-145.11	24.92	24.92
8.00	-145.24	24.96	24.96
8.33	-145.30	25.00	25.00
8.67	-145.40	25.02	25.02
9.00	-145.52	25.01	25.01
9.33	-145.60	25.00	25.00
9.67	-145.61	25.00	25.00

EFFECTIVE POTENTIAL FOR OMEGA = -75.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.10	0.01	0.02
0.67	-0.24	0.04	0.05
1.00	-0.56	0.08	0.10
1.33	-1.29	0.19	0.22
1.67	-2.83	0.41	0.47
2.00	-5.87	0.85	0.93
2.33	-11.32	1.65	1.75
2.67	-20.11	3.00	3.10
3.00	-32.67	5.05	5.11
3.33	-48.56	7.81	7.82
3.67	-66.53	11.12	11.07
4.00	-84.83	14.61	14.50
4.33	-101.77	17.83	17.70
4.67	-116.06	20.41	20.28
5.00	-127.07	22.22	22.12
5.33	-134.85	23.37	23.30
5.67	-139.90	24.06	24.03
6.00	-142.97	24.52	24.51
6.33	-144.86	24.85	24.85
6.67	-146.11	25.06	25.07
7.00	-147.01	25.17	25.18
7.33	-147.60	25.22	25.22
7.67	-147.92	25.24	25.24
8.00	-148.05	25.28	25.28
8.33	-148.12	25.32	25.33
8.67	-148.22	25.34	25.34
9.00	-148.34	25.34	25.34
9.33	-148.41	25.33	25.33
9.67	-148.42	25.33	25.33

EFFECTIVE POTENTIAL FOR OMEGA = -60.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.10	0.02	0.02
0.67	-0.24	0.04	0.05
1.00	-0.58	0.09	0.11
1.33	-1.32	0.19	0.23
1.67	-2.90	0.42	0.48
2.00	-6.00	0.87	0.95
2.33	-11.58	1.70	1.79
2.67	-20.57	3.09	3.17
3.00	-33.41	5.18	5.23
3.33	-49.69	8.00	8.00
3.67	-68.10	11.36	11.31
4.00	-86.87	14.91	14.81
4.33	-104.22	18.17	18.05
4.67	-118.80	20.79	20.67
5.00	-129.99	22.61	22.52
5.33	-137.85	23.76	23.70
5.67	-142.94	24.46	24.43
6.00	-146.04	24.92	24.91
6.33	-147.95	25.24	25.25
6.67	-149.22	25.46	25.46
7.00	-150.12	25.57	25.57
7.33	-150.72	25.61	25.61
7.67	-151.03	25.64	25.64
8.00	-151.17	25.68	25.68
8.33	-151.25	25.72	25.72
8.67	-151.35	25.74	25.74
9.00	-151.46	25.73	25.73
9.33	-151.53	25.72	25.72
9.67	-151.54	25.72	25.72

EFFECTIVE POTENTIAL FOR OMEGA = -45.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.10	0.02	0.02
0.67	-0.25	0.04	0.05
1.00	-0.60	0.09	0.11
1.33	-1.36	0.20	0.24
1.67	-2.98	0.44	0.49
2.00	-6.18	0.91	0.98
2.33	-11.90	1.77	1.85
2.67	-21.12	3.19	3.27
3.00	-34.31	5.34	5.38
3.33	-51.03	8.23	8.22
3.67	-69.96	11.68	11.62
4.00	-89.25	15.29	15.20
4.33	-107.04	18.60	18.50
4.67	-121.95	21.25	21.16
5.00	-133.32	23.10	23.02
5.33	-141.26	24.25	24.19
5.67	-146.38	24.95	24.91
6.00	-149.52	25.40	25.39
6.33	-151.45	25.73	25.73
6.67	-152.73	25.94	25.95
7.00	-153.64	26.05	26.05
7.33	-154.23	26.09	26.09
7.67	-154.54	26.12	26.11
8.00	-154.68	26.15	26.16
8.33	-154.77	26.20	26.20
8.67	-154.87	26.22	26.22
9.00	-154.98	26.21	26.21
9.33	-155.04	26.20	26.19
9.67	-155.05	26.20	26.20

EFFECTIVE POTENTIAL FOR OMEGA = -30.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.04	0.01	0.01
0.33	-0.11	0.02	0.02
0.67	-0.26	0.04	0.05
1.00	-0.62	0.09	0.11
1.33	-1.42	0.21	0.25
1.67	-3.10	0.46	0.52
2.00	-6.40	0.96	1.02
2.33	-12.31	1.85	1.93
2.67	-21.83	3.34	3.40
3.00	-35.44	5.57	5.59
3.33	-52.70	8.55	8.52
3.67	-72.23	12.09	12.03
4.00	-92.12	15.79	15.71
4.33	-110.41	19.17	19.09
4.67	-125.66	21.85	21.78
5.00	-137.22	23.71	23.65
5.33	-145.23	24.86	24.81
5.67	-150.38	25.56	25.52
6.00	-153.53	26.01	26.00
6.33	-155.48	26.33	26.34
6.67	-156.78	26.54	26.55
7.00	-157.68	26.65	26.65
7.33	-158.26	26.69	26.69
7.67	-158.57	26.71	26.71
8.00	-158.72	26.75	26.75
8.33	-158.81	26.79	26.80
8.67	-158.92	26.81	26.82
9.00	-159.02	26.81	26.81
9.33	-159.08	26.80	26.79
9.67	-159.09	26.80	26.80

EFFECTIVE POTENTIAL FOR OMEGA = -15.00 MEV

Z	V ZERO	V PERP	V PARL
0.	-0.05	0.01	0.01
0.33	-0.12	0.02	0.02
0.67	-0.28	0.04	0.05
1.00	-0.65	0.10	0.12
1.33	-1.49	0.23	0.26
1.67	-3.25	0.50	0.55
2.00	-6.71	1.03	1.09
2.33	-12.88	1.98	2.04
2.67	-22.80	3.55	3.59
3.00	-36.95	5.89	5.89
3.33	-54.90	9.00	8.96
3.67	-75.18	12.67	12.61
4.00	-95.77	16.48	16.42
4.33	-114.63	19.94	19.88
4.67	-130.23	22.66	22.61
5.00	-141.96	24.53	24.48
5.33	-150.02	25.67	25.62
5.67	-155.16	26.35	26.31
6.00	-158.31	26.79	26.78
6.33	-160.28	27.11	27.12
6.67	-161.58	27.32	27.34
7.00	-162.48	27.42	27.43
7.33	-163.05	27.46	27.46
7.67	-163.35	27.49	27.48
8.00	-163.50	27.52	27.52
8.33	-163.61	27.57	27.57
8.67	-163.71	27.59	27.59
9.00	-163.81	27.58	27.58
9.33	-163.86	27.57	27.56
9.67	-163.88	27.57	27.56

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5. The Fourier time transform of Eqs. (2.14) and (4.40) include a term containing μ in the exponent which is not used in the analogous equations in references 2 through 4. This discrepancy produces a change in the ω -dependence of the spectral function $A(\omega)$ and (in the Puff-Martin case) of the effective potential $V(p\omega)$:

$$A_{\text{present}}(\omega) = A_{\text{ref } 2-4}(\omega - \mu);$$

$$V_{\text{present}}(\omega) = V_{\text{ref } 2-4}(\omega - \mu).$$

This discrepancy in V extends to the effective-mass coefficients V_0 , V_{\perp} , and V_{\parallel} (or to V_0 and V_2 in the homogeneous case). Note also that V is called Σ (self energy) in references 3 and 4.

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15. This fact was learned through painful experience. Originally, the entire computation described in the next chapter was carried out for the μ zero point. The final iterative computation did not converge but, instead, led to a situation in which each result for the effective potential reproduced the result of the previous iteration displaced along the Z-axis (towards the vacuum side) by about $\frac{1}{4}$ fermi. Further calculations suggested that a time-independent solution did not exist. Only at this point was the distinction between the various zero points realized and the local-transport zero point derived and shown to be appropriate.
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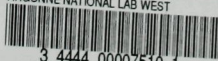
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Most of the computations were done on IBM 704 and 709 computers at Argonne and at the Massachusetts Institute of Technology Computation Center. A few computations were done on a commercial IBM 704 with the aid of funds from the Office of Scientific Research of the U. S. Air Force. The programming was done largely in Fortran.

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